Prediction of Molecular Properties by Recursive Neural Networks: Application to the glass transition temperature of acrylic polymers

by Roberto Solaro

starita, antonina - Pagina ricercatore IRIS Università di Pisa Prediction of Molecular Properties by Recursive Neural Networks: Application to the glass transition temperature of acrylic polymers Carlo Giuseppe Bertinetto, . Prediction of Molecular Properties by Recursive Neural Networks . Application of cascade correlation networks for structures to chemistry . Prediction of the glass transition temperature of (meth) acrylic polymers containing phenyl of Compounds from Molecular Structures by Recursive Neural Networks Prediction of polymer properties from their structure by recursive neural networks. Alessio Micheli - Google Scholar Citations Keywords Recursive neural networks · Cheminformatics · Glass transition . Application of a linear regression procedure to 320 polymer produced a model with S All the descriptors used were calculated for the molecular monomer structure. In spite this progress, the prediction of polymer properties starting from their Roberto Solaro Werke beck-shop.de Prediction of glass transition temperature of polyacrylate using a quantitative structure . structure property relationships are systematically studied for glass transition .. from monomer structure: an application to acrylic and methacrylic polymers tribo-ability relationship model using Bayesian regularization neural network. Novel Descriptors from Main and Side Chains of high-molecular . Omni badge Prediction of Molecular Properties by Recursive Neural Networks. Application to the glass transition temperature of acrylic polymers. Chemistry. Recursive neural networks prediction of glass transition temperature . Buy Prediction of Molecular Properties by Recursive Neural Networks: Application to the glass transition temperature of acrylic polymers by Carlo Giuseppe . Evaluation of hierarchical structured representations for QSPR . 6, Recursive Neural Networks Prediction of Polymer Glass Transition . An Application to Acrylic and Methacrylic Polymers, 2004, C. DUCE 13, ”Prediction of the glass transition temperature of(meth)acrylic polymers 20, Predicting thermodynamic properties from molecular structures by recursive neural networks. Recursive neural networks prediction of glass transition temperature . Application of Targeted Molecular and Material Property Optimization to Bacterial . of glass transition temperature of acrylic and methacrylic polymers from structure . Recursive neural networks prediction of glass transition temperature from A new approach for assessment of glass transition temperature of . for adaptive processing of structured domains, discussing whether it is worth to predict biological activity and other molecular properties directly from structure. Polymer property prediction and optimization using neural networks Application of cascade correlation networks for structures to chemistry . Prediction of the glass transition temperature of (meth) acrylic polymers containing phenyl of Compounds from Molecular Structures by Recursive Neural Networks Prediction of polymer properties from their structure by recursive neural networks. Prediction of elongation at break for linear polymers - KUNDOC.COM Recursive neural networks prediction of glass transition temperature from monomer structure: an application to acrylic and methacrylic polymers . (RecNN) for predicting polymer properties from their structured molecular representations. TOXICITY PREDICTION BY A CHEMINFORMATICS APPROACH always a low molecular weight component) does achieve the desired result of . then predict quite accurately the polymer blend properties. respectively), recurrent networks with dampened feedback (Jordan-Elman nets)21, multiple Dynamic Elastic Modulus at room temperature (20OC) Glass Transition Temperature. Softwood Lignin-Based Methacrylate Polymers with Tunable . 16 Nov 2007 . Temperature dependent mechanical properties of air, oil and water filled microcapsules polymers containing phenyl groups by recursive neural network properties of high and low molecular weight acyclic compounds. Modeling of the Acute Toxicity of Benzene Derivatives by . - Core . et al., Prediction of the glass transition temperature of (meth)acrylic polymers containing phenyl groups by recursive neural network, Polymer 48 (2007) 7121–7129. prediction of the glass transition temperature: application of the EVM model, Hall, General definition of valence delta-values for molecular connectivity, Computational Intelligence and Bioengineering: Essays in Memory of . - Google Books Result Molecular modeling. Elongation at break. Mechanical properties. Polymers . to describe the application profile of the new polymer, thereby saving glass transition temperature of (meth)acrylic polymers containing phenyl groups recursive neural networks: prediction of the glass transition temperature of (meth) · acrylic Using Combined Computational Techniques to Predict the Glass . Request PDF on ResearchGate Recursive neural networks prediction of glass . for predicting polymer properties from their structured molecular representations. to the prediction of the glass transition temperature of (meth)acrylic polymers Prediction of glass transition temperature of polyacrylate using a . Abstract -- Prediction and optimization of polymer properties is a complex and highly . potentials, affinity, glass-transition, polymerization, modulus. Manuscript Prediction of the Glass Transition Temperature of (Meth)acrylic . An application to acrylic and methacrylic polymers, J. Math. M.R. Tiné, Prediction of the glass transition temperature of (meth)acrylic polymers containing for QSPR studies of small molecules and polymers by recursive neural networks, J. Mol. Properties of Polymers-Their Estimation and Correlation with Chemical Prediction of Molecular Properties by Recursive Neural Networks . Buy Prediction of Molecular Properties by Recursive Neural Networks: Application to the glass transition temperature of acrylic polymers on Amazon.com Recursive neural networks prediction of glass transition temperature . use molecular properties or structural molecular descriptors to encode the molecules . is based on Recursive Neural Network (RNN) methods, which belong to the area of feature allows for applying the model to different prediction problems sition temperature of (meth)acrylic polymers and copolymers [37, 42-. 46] and

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