QSAR Prediction Reporting Format (QPRF) for the Vapour pressure of NaTFSI estimated with MPBPVP

1. Substance

1.1 CAS number: 91742-21-1

1.2 EC number: Not yet assigned

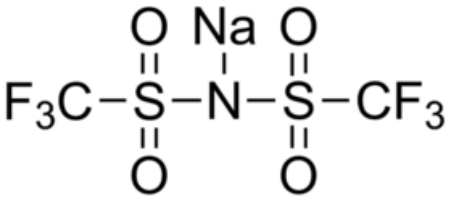
1.3 Chemical name: Sodium bis(trifluoromethylsulfonyl)imide

1.4 Synonym: NaTFSI

1.5 Molecular formula: $C_2F_6NNaO_4S_2$

1.6 Molecular weight: 303.14 g/mol

1.7 Structural formula:



1.8 Structure codes:

a. **SMILES**: FC(F)(F)S(=O)(=O)N([Na])S(=O)(=O)C(F)(F)F

b. **InChI:** 1S/C2F6NO4S2.Na/c3-1(4,5)14(10,11)9-15(12,13)2(6,7)8;/q-1;+1

c. **Other structural representation**: Not available.

d. **Stereochemical features:** The substance is not a stereoisomer.

2. General information

2.1 Date of QPRF: March 12nd 2021

2.2 QPRF author and contact details:

Solvay S.A. – HSE - TERA
Rue de Ransbeek, 310
1120 Brussels

3. Prediction

3.1 Endpoint (OECD Principle 1)

a. **Endpoint**: Physical-chemical parameters – Vapour Pressure

b. **Dependant variable:** Vapour pressure (Pa)

3.2 Algorithm (OECD Principle 2)

a. **Model or submodel name:** US EPA On-Line EPI SuiteTM, MPBPVP v 1.43

b. **Model version:** MPBPVP v1.43, part of EPIWeb 4.11 suite, U.S EPA. 2012. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. United States Environmental Protection Agency, Washington, DC, USA.

c. **Reference to QMRF:** The corresponding QMRF named 'QSAR Model

Reporting Format: Use of quantitative structure-activity relationships in REACH compliance – Prediction of vapour pressure – Modified Grain method' has been compiled.

d. **Predicted value (model result):** Selected VP = 6.01E-009 Pa

e. **Predicted value (comments):** None

f. **Input for prediction:** SMILES as described in section 1.8 was used to generate the prediction. Boiling point: 525.5°C; Melting point: 224.5°C.

g. **Descriptor value:** None

3.3 Applicability domain (OECD principle 3)

Currently there is no universally accepted definition of model domain. However, the estimates may be less accurate for compounds outside the MW range of the training set compounds, and/or that have more instances of a given fragment than the maximum for all training/validation set compounds can be considered. It is also possible that a compound may have a functional group(s) or other structural features not represented in the training/validation set, and for which no fragment coefficient was developed. These points should be taken into consideration when interpreting model results.

a. **Domains:** The substance was found to fall in the applicability domain of the model

b. No structural analogues present in the training and test sets

c. **Considerations on structural analogues:** Not applicable

3.4 The uncertainty of the prediction (OECD principle 4)

The general accurate performance of the MPBPVP prediction of vapour pressure is demonstrated by the standard deviation of 1.06 (r^2 = 0.914, n = 3037). However the accuracy of the estimate using this method has been demonstrated to decrease with decreasing value of VP, showing greater scatter in the data set, particularly below 1E-04 Pa.

3.5 The chemical and biological mechanisms according to the model underpinning the predicted result (OECD principle 5).

The derivation of vapour pressure based on the physical state and boiling point, as used by this algorithm, is well established for organic chemicals.

4. Adequacy (Optional)

4.1 Regulatory purpose: The prediction is to be used for Registration of the substance under the REACH regulation.

4.2 Approach for regulatory interpretation of the model result: Vapour pressure is a required endpoint under Annex VII of the REACH regulation. No further processing of the result is needed for this purpose.

4.3 Outcome: VP = 6.01E-009 Pa.

4.4 Conclusion: The accuracy of the prediction is considered sufficient for the regulatory purpose.