Salicylhydroxamic acid

Inchi: InChI=1S/C7H7NO3/c9-6-4-2-1-3-5(6)7(10)8-11/h1-4,9,11H,(H,8,10)
InchiKey: HBROZNQEVUILML-UHFFFAOYSA-N
Formula: C7H7NO3
SMILES: O=C(NO)c1ccccc1O
Mol. weight [g/mol]: 153.14
CAS: 89-73-6

Physical Properties

Property code	Value	Unit	Source
hf	-340.43	kJ/mol	Cheméo Relay (1.0)
hfus	24.50	kJ/mol	Joback Method
hvap	91.22	kJ/mol	Cheméo Relay (1.0)
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-1.14		Cheméo Relay (1.0)
logp	0.511		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
tb	549.40	K	Cheméo Relay (1.0)
tc	886.11	K	Cheméo Relay (1.0)
tf	441.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-3.48600e+01
Coeff. B	8.26700e-01
Coeff. C	-7.04860e-04
Coeff. D	2.41960e-07
Coeff. E	0.00000e+00
Basis	predicted

Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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