6-Hydroxy-2-naphthoic acid

Inchi: InChI=1S/C11H8O3/c12-10-4-3-7-5-9(11(13)14)2-1-8(7)6-10/h1-6,12H,(H,13,14)
InchiKey: KAUQJMHLAFIZDU-UHFFFAOYSA-N
Formula: C11H8O3
SMILES: O=C(O)c1ccc2cc(O)ccc2c1
Mol. weight [g/mol]: 188.18
CAS: 16712-64-4

Physical Properties

Property code	Value	Unit	Source
hf	-400.01	kJ/mol	Cheméo Relay (1.0)
hfus	30.84	kJ/mol	Joback Method
hvap	123.18	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	Cheméo Relay (1.0)
log10ws	-2.75		Cheméo Relay (1.0)
logp	2.244		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
tb	629.30	K	Cheméo Relay (1.0)
tf	522.15	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	-6.24800e+01
Coeff. B	1.11210e+00
Coeff. C	-1.00444e-03
Coeff. D	3.62500e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.64206e+01
Coeff. B	4.31252e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	522.15
Temperature range (K), max.	686.58

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

tf: Normal melting (fusion) point

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