1-Amino-8-naphthol-3,6-disulfonic acid

Other names: 4-amino-5-hydroxynaphthalene-2,7-disulphonic acid
Inchi: InChI=1S/C10H9NO7S2/c11-8-3-6(19(13,14)15)1-5-2-7(20(16,17)18)4-9(12)10(5)8/h1-4,
InchiKey: APRRQJCCBSJQOQ-UHFFFAOYSA-N
Formula: C10H9NO7S2
SMILES: Nc1cc(S(=O)(=O)O)cc2cc(S(=O)(=O)O)cc(O)c12
Mol. weight [g/mol]: 319.31
CAS: 90-20-0

Physical Properties

Property code	Value	Unit	Source
gf	-1075.40	kJ/mol	Joback Method
hf	-1211.22	kJ/mol	Joback Method
hfus	53.46	kJ/mol	Joback Method
hvap	138.04	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	0.621		Crippen Method
mcvol	192.310	ml/mol	McGowan Method
pc	11150.65	kPa	Joback Method
tb	921.87	K	Joback Method
tc	1139.04	K	Joback Method
tf	692.88	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.64	J/mol×K	921.87	Joback Method
cpg	544.68	J/mol×K	958.06	Joback Method
cpg	550.17	J/mol×K	994.26	Joback Method
cpg	555.18	J/mol×K	1030.45	Joback Method
cpg	559.74	J/mol×K	1066.65	Joback Method
cpg	563.90	J/mol×K	1102.84	Joback Method
cpg	567.73	J/mol×K	1139.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90200&Units=SI

Legend

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