

1-Naphthalenesulfonic acid,4-amino-3-hydroxy-

Other names:1-Amino-2-naphthol-4-sulfonic acid
4-amino-3-hydroxynaphthalene-1-sulphonic acid

Inchi:InChI=1S/C10H9NO4S/c11-10-7-4-2-1-3-6(7)9(5-8(10)12)16(13,14)15/h1-5,12H,11H2,(H

InchiKey:RXCMFQDTWCCLBL-UHFFFAOYSA-N

Formula:C10H9NO4S

SMILES:Nc1c(O)cc(S(=O)(=O)O)c2cccc12

Mol. weight [g/mol]:239.25

CAS:116-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-460.41	kJ/mol	Joback Method
hf	-594.17	kJ/mol	Joback Method
hfus	38.38	kJ/mol	Joback Method
hvap	102.06	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.374		Crippen Method
mcvol	158.350	ml/mol	McGowan Method
pc	7194.03	kPa	Joback Method
tb	776.93	K	Joback Method
tc	1003.89	K	Joback Method
tf	580.98	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.88	J/mol×K	776.93	Joback Method
cpg	432.15	J/mol×K	814.76	Joback Method
cpg	439.85	J/mol×K	852.58	Joback Method
cpg	447.09	J/mol×K	890.41	Joback Method
cpg	453.93	J/mol×K	928.24	Joback Method
cpg	460.47	J/mol×K	966.07	Joback Method
cpg	466.78	J/mol×K	1003.89	Joback Method

Sources

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=C116632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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