

1,7-Cleve's acid

Other names:	8-Amino-2-naphthalenesulfonic acid 8-Aminonaphthalene-2-sulfonic acid 1-Naphthylamine-7-sulfonic acid 1-Amino-7-naphthalenesulfonic acid 2-Naphthalenesulfonic acid, 8-amino- C.I. 26135 Cleve's theta-acid 1-Amino-7-sulfonaphthalene 1-Aminonaphthalene-7-sulfonic acid 8-Naphthylamine-2-sulfonic acid «alpha»-Naphthylamine 7-sulfonic acid NSC 4983 1-Naphthylamino-7-sulfonic acid 8-aminonaphthalene-2-sulphonic acid
Inchi:	InChI=1S/C10H9NO3S/c11-10-3-1-2-7-4-5-8(6-9(7)10)15(12,13)14/h1-6H,11H2,(H,12,13)
InchiKey:	QEZCWMQXHXAFG-UHFFFAOYSA-N
Formula:	C10H9NO3S
SMILES:	Nc1cccc2ccc(S(=O)(=O)O)cc12
Mol. weight [g/mol]:	223.25
CAS:	119-28-8

Physical Properties

Property code	Value	Unit	Source
gf	-305.79	kJ/mol	Joback Method
hf	-416.86	kJ/mol	Joback Method
hfus	32.60	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.669		Crippen Method
mcvol	152.480	ml/mol	McGowan Method
pc	5670.27	kPa	Joback Method
tb	696.31	K	Joback Method
tc	915.54	K	Joback Method
tf	469.26	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.65	J/mol×K	696.31	Joback Method
cpg	394.35	J/mol×K	732.85	Joback Method
cpg	403.26	J/mol×K	769.39	Joback Method
cpg	411.43	J/mol×K	805.93	Joback Method
cpg	418.88	J/mol×K	842.47	Joback Method
cpg	425.66	J/mol×K	879.00	Joback Method
cpg	431.79	J/mol×K	915.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119288&Units=SI
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

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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