

1-AMINOPHTHALENE-6-SULPHONIC ACID

Other names:	1-Amino-6-naphthalenesulfonic acid 1-Amino-6-sulfonaphthalene 1-Aminonaphthalene-6-sulfonic acid 1-Naphthylamine-6-sulfonic acid 2-Naphthalenesulfonic acid, 5-amino- 5-Amino-2-naphthalenesulfonic acid 5-Naphthylamine-2-sulfonic acid 5-aminonaphthalene-2-sulphonic acid Cleve's acid-1,6 Cleve's «beta»-acid Kyselina 1-naftylamin-6-sulfonova Kyselina cleve NSC 31506 «alpha»-Naphthylamine-6-sulfonic acid
Inchi:	InChI=1S/C10H9NO3S/c11-10-3-1-2-7-6-8(15(12,13)14)4-5-9(7)10/h1-6H,11H2,(H,12,13)
InchiKey:	UWPJYQYRSWYIGZ-UHFFFAOYSA-N
Formula:	C10H9NO3S
SMILES:	Nc1cccc2cc(S(=O)(=O)O)ccc12
Mol. weight [g/mol]:	223.25

Physical Properties

Property code	Value	Unit	Source
hfus	32.60	kJ/mol	Joback Method
hvap	132.65	kJ/mol	Cheméo Relay (1.0)
ie	7.85	eV	Cheméo Relay (1.0)
log10ws	-1.25		Cheméo Relay (1.0)
logp	1.669		Crippen Method
mcvol	152.480	ml/mol	McGowan Method
tb	670.25	K	Cheméo Relay (1.0)
tf	539.85	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119799&Units=SI
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
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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