

2-Chloro-5-nitrobenzene sulfonic acid

Other names:	2-chloro-5-nitrobenzenesulphonic acid
Inchi:	InChI=1S/C6H4ClNO5S/c7-5-2-1-4(8(9)10)3-6(5)14(11,12)13/h1-3H,(H,11,12,13)
InchiKey:	GNTARUIZNIWBCN-UHFFFAOYSA-N
Formula:	C6H4ClNO5S
SMILES:	O=[N+]([O-])c1ccc(Cl)c(S(=O)(=O)O)c1
Mol. weight [g/mol]:	237.62
CAS:	96-73-1

Physical Properties

Property code	Value	Unit	Source
gf	-488.95	kJ/mol	Joback Method
hf	-585.66	kJ/mol	Joback Method
hfus	35.58	kJ/mol	Joback Method
hvap	88.84	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.495		Crippen Method
mcvol	135.260	ml/mol	McGowan Method
pc	6190.26	kPa	Joback Method
tb	702.55	K	Joback Method
tc	929.06	K	Joback Method
tf	481.75	K	Joback Method
vc	0.539	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.15	J/mol×K	702.55	Joback Method
cpg	316.22	J/mol×K	740.30	Joback Method
cpg	322.61	J/mol×K	778.05	Joback Method
cpg	328.33	J/mol×K	815.81	Joback Method
cpg	333.38	J/mol×K	853.56	Joback Method
cpg	337.76	J/mol×K	891.31	Joback Method
cpg	341.47	J/mol×K	929.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C96731&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
h vap:	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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