m-Nitrobenzensulfonic acid

Other names:	m-Nitrobenzenesulfonic acid
	3-Nitrobenzenesulfonic acid
	Benzenesulfonic acid, 3-nitro-
	Benzenesulfonic acid, m-nitro-
	Kyselina nitrobenzen-m-sulfonova
	Kyselina 3-nitrobenzensulfonova
	3-nitrobenzenesulphonic acid
Inchi:	InChI=1S/C6H5NO5S/c8-7(9)5-2-1-3-6(4-5)13(10,11)12/h1-4H,(H,10,11,12)
InchiKey:	ONMOULMPIIOVTQ-UHFFFAOYSA-N
Formula:	C6H5NO5S
SMILES:	O=[N+]([O-])c1cccc(S(=O)(=O)O)c1
Mol. weight [g/mol]:	203.17
CAS:	98-47-5

Physical Properties

Property code	Value	Unit	Source
gf	-467.39	kJ/mol	Joback Method
hf	-558.45	kJ/mol	Joback Method
hfus	31.78	kJ/mol	Joback Method
hvap	83.79	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	0.842		Crippen Method
mcvol	123.020	ml/mol	McGowan Method
pc	6729.65	kPa	Joback Method
tb	660.14	K	Joback Method
tc	882.84	K	Joback Method
tf	439.31	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.23	J/mol×K	660.14	Joback Method
cpg	300.37	J/mol×K	697.26	Joback Method

cpg	307.81	J/mol×K	734.37	Joback Method
cpg	314.56	J/mol×K	771.49	Joback Method
cpg	320.63	J/mol×K	808.61	Joback Method
cpg	326.03	J/mol×K	845.73	Joback Method
cpg	330.76	J/mol×K	882.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98475&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