4-Chloro-N-(2-methyl-4-nitrophenyl)-benzenesulfo N-methyl-

Inchi: InChI=1S/C14H13ClN2O4S/c1-10-9-12(17(18)19)5-8-14(10)16(2)22(20,21)13-6-3-11(15)

InchiKey: MXBOECKBBXIUOS-UHFFFAOYSA-N

Formula: C14H13ClN2O4S

SMILES: Cc1cc([N+](=O)[O-])ccc1N(C)S(=O)(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 340.78

Physical Properties

Property code	Value	Unit	Source
gf	-71.21	kJ/mol	Joback Method
hf	-305.96	kJ/mol	Joback Method
hfus	48.89	kJ/mol	Joback Method
hvap	94.95	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.382		Crippen Method
mcvol	228.330	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	2683.00		NIST Webbook
tb	837.51	K	Joback Method
tc	1086.13	K	Joback Method
tf	582.50	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.09	J/mol×K	837.51	Joback Method
cpg	630.71	J/mol×K	878.95	Joback Method
cpg	640.99	J/mol×K	920.38	Joback Method
cpg	649.98	J/mol×K	961.82	Joback Method
cpg	657.76	J/mol×K	1003.26	Joback Method
cpg	664.37	J/mol×K	1044.69	Joback Method
cpg	669.87	J/mol×K	1086.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume