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

Inchi: InChI=1S/C13H11ClN2O4S/c1-9-8-11(16(17)18)4-7-13(9)15-21(19,20)12-5-2-10(14)3-6-
InchiKey: CNZQESBPARGYEP-UHFFFAOYSA-N
Formula: C13H11ClN2O4S
SMILES: Cc1cc([N+](=O)[O-])ccc1NS(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 326.75
CAS: 10589-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-101.02	kJ/mol	Joback Method
hf	-299.38	kJ/mol	Joback Method
hfus	48.38	kJ/mol	Joback Method
hvap	97.12	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.357		Crippen Method
mcvol	214.240	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	2757.00		NIST Webbook
rinpol	2757.00		NIST Webbook
tb	852.36	K	Joback Method
tc	1106.31	K	Joback Method
tf	591.42	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.15	J/mol×K	852.36	Joback Method
cpg	584.46	J/mol×K	894.69	Joback Method
cpg	593.44	J/mol×K	937.01	Joback Method
cpg	601.15	J/mol×K	979.34	Joback Method
cpg	607.62	J/mol×K	1021.66	Joback Method
cpg	612.90	J/mol×K	1063.99	Joback Method
cpg	617.03	J/mol×K	1106.31	Joback Method

Sources

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=C10589647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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