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

Inchi: InChI=1S/C15H10ClF3N2O5S/c1-9-8-11(21(23)24)4-7-13(9)20(14(22)15(17,18)19)27(25
InchiKey: YLDNZOAGXIBEPS-UHFFFAOYSA-N
Formula: C15H10ClF3N2O5S
SMILES: Cc1cc([N+](=O)[O-])ccc1N(C(=O)C(F)(F)F)S(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 422.76

Physical Properties

Property code	Value	Unit	Source
gf	-773.30	kJ/mol	Joback Method
hf	-1036.26	kJ/mol	Joback Method
hfus	54.90	kJ/mol	Joback Method
hvap	100.17	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	3.841		Crippen Method
mcvol	249.300	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	2472.00		NIST Webbook
tb	908.84	K	Joback Method
tc	1144.15	K	Joback Method
tf	647.89	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.59	J/mol×K	908.84	Joback Method
cpg	711.01	J/mol×K	948.06	Joback Method
cpg	718.33	J/mol×K	987.28	Joback Method
cpg	724.63	J/mol×K	1026.50	Joback Method
cpg	729.99	J/mol×K	1065.71	Joback Method
cpg	734.50	J/mol×K	1104.93	Joback Method
cpg	738.23	J/mol×K	1144.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374788&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume