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

Inchi: InChI=1S/C16H10ClF5N2O5S/c1-9-8-11(24(26)27)4-7-13(9)23(14(25)15(18,19)16(20,21
InchiKey: YWEVIRDQFMLLJA-UHFFFAOYSA-N
Formula: C16H10ClF5N2O5S
SMILES: Cc1cc([N+](=O)[O-])ccc1N(C(=O)C(F)(F)C(F)(F)F)S(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 472.77

Physical Properties

Property code	Value	Unit	Source
gf	-1151.66	kJ/mol	Joback Method
hf	-1457.87	kJ/mol	Joback Method
hfus	56.24	kJ/mol	Joback Method
hvap	99.47	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	4.476		Crippen Method
mcvol	266.930	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
tb	927.03	K	Joback Method
tc	1155.66	K	Joback Method
tf	662.76	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.10	J/mol×K	927.03	Joback Method
cpg	781.16	J/mol×K	965.13	Joback Method
cpg	788.25	J/mol×K	1003.24	Joback Method
cpg	794.49	J/mol×K	1041.34	Joback Method
cpg	799.98	J/mol×K	1079.45	Joback Method
cpg	804.84	J/mol×K	1117.55	Joback Method
cpg	809.16	J/mol×K	1155.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374789&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

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