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

InChI: InChI=1S/C17H10ClF7N2O5S/c1-9-8-11(27(29)30)4-7-13(9)26(33(31,32)12-5-2-10(18)3
InChIKey: PEXLMSOGCTYPOV-UHFFFAOYSA-N
Formula: C17H10ClF7N2O5S
SMILES: Cc1cc([N+](=O)[O-])ccc1N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)S(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 522.78

Physical Properties

Property code	Value	Unit	Source
gf	-1530.02	kJ/mol	Joback Method
hf	-1879.48	kJ/mol	Joback Method
hfus	57.57	kJ/mol	Joback Method
hvap	98.77	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.111		Crippen Method
mcvol	284.560	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2417.00		NIST Webbook
tb	945.22	K	Joback Method
tc	1169.36	K	Joback Method
tf	677.63	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.71	J/mol×K	945.22	Joback Method
cpg	851.52	J/mol×K	982.58	Joback Method
cpg	858.52	J/mol×K	1019.93	Joback Method
cpg	864.83	J/mol×K	1057.29	Joback Method
cpg	870.58	J/mol×K	1094.65	Joback Method
cpg	875.91	J/mol×K	1132.00	Joback Method
cpg	880.94	J/mol×K	1169.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374790&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