N-(3-Chlorophenyl)-N-(2,2,3,3,4,4,4-heptafluorobu

Inchi: InChI=1S/C14H4ClF14NO2/c15-5-2-1-3-6(4-5)30(7(31)9(16,17)11(20,21)13(24,25)26)8(
InchiKey: IFIUOBAHQVAEDB-UHFFFAOYSA-N
Formula: C14H4ClF14NO2
SMILES: O=C(N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1cccc(Cl)c1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 519.62

Physical Properties

Property code	Value	Unit	Source
gf	-2699.51	kJ/mol	Joback Method
hf	-3078.64	kJ/mol	Joback Method
hfus	34.72	kJ/mol	Joback Method
hvap	50.40	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.865		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	1201.00		NIST Webbook
tb	679.39	K	Joback Method
tc	847.23	K	Joback Method
tf	471.51	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.61	J/mol×K	679.39	Joback Method
cpg	691.06	J/mol×K	707.36	Joback Method
cpg	699.58	J/mol×K	735.34	Joback Method
cpg	707.28	J/mol×K	763.31	Joback Method
cpg	714.25	J/mol×K	791.28	Joback Method
cpg	720.57	J/mol×K	819.25	Joback Method
cpg	726.35	J/mol×K	847.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373272&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