N-(5-Chloro-2-methyl-phenyl)-2,2,3,3,4,4,4-heptafl

Inchi: InChI=1S/C11H7ClF7NO/c1-5-2-3-6(12)4-7(5)20-8(21)9(13,14)10(15,16)11(17,18)19/h2-
InchiKey: QBCVQCFMEVMUBF-UHFFFAOYSA-N
Formula: C11H7ClF7NO
SMILES: Cc1ccc(Cl)cc1NC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 337.62

Physical Properties

Property code	Value	Unit	Source
gf	-1271.72	kJ/mol	Joback Method
hf	-1530.65	kJ/mol	Joback Method
hfus	27.72	kJ/mol	Joback Method
hvap	51.64	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.420		Crippen Method
mcvol	178.270	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
tb	614.39	K	Joback Method
tc	801.93	K	Joback Method
tf	409.09	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.78	J/mol×K	614.39	Joback Method
cpg	474.52	J/mol×K	645.65	Joback Method
cpg	484.38	J/mol×K	676.90	Joback Method
cpg	493.42	J/mol×K	708.16	Joback Method
cpg	501.71	J/mol×K	739.42	Joback Method
cpg	509.30	J/mol×K	770.68	Joback Method
cpg	516.28	J/mol×K	801.93	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=U373249&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