N-(3-Chlorophenyl)-bis(2,2,3,3,3-pentafluoropropa

Other names: N-(3-Chlorophenyl)-2,2,3,3,3-pentafluoro-N-(2,2,3,3,3-pentafluoro-propionyl)propionamid
Inchi: InChI=1S/C12H4ClF10NO2/c13-5-2-1-3-6(4-5)24(7(25)9(14,15)11(18,19)20)8(26)10(16,
InchiKey: FROKFCZQWJECDZ-UHFFFAOYSA-N
Formula: C12H4ClF10NO2
SMILES: O=C(N(C(=O)C(F)(F)C(F)(F)F)c1cccc(Cl)c1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 419.60

Physical Properties

Property code	Value	Unit	Source
gf	-1942.79	kJ/mol	Joback Method
hf	-2235.42	kJ/mol	Joback Method
hfus	32.05	kJ/mol	Joback Method
hvap	51.81	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.595		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
tb	643.01	K	Joback Method
tc	819.70	K	Joback Method
tf	441.77	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.57	J/mol×K	643.01	Joback Method
cpg	553.29	J/mol×K	672.46	Joback Method
cpg	562.10	J/mol×K	701.91	Joback Method
cpg	570.08	J/mol×K	731.36	Joback Method
cpg	577.30	J/mol×K	760.81	Joback Method
cpg	583.85	J/mol×K	790.25	Joback Method
cpg	589.81	J/mol×K	819.70	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=U378226&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