N-(2-Chloro-4-(3-chloro-4-[(2,2,3,3,3-pentafluoropr

Other names:	N-[2-Chloro-4-[[3-chloro-4-[(2,2,3,3,3-pentafluoropropionyl)amino]phenyl]methyl]phenyl]-b
	Propionylamide,
	N,N'-[methylenebis(2-chloro-4,1-phenylene)]bis[2,2,3,3,3-pentafluoro-
	N,N'-[Methanediylbis(2-chlorobenzene-4,1-diyl)]tris(2,2,3,3,3-pentafluoropropionylamide)
	N,N'-[Methylenebis(2-chloro-4,1-phenylene)]tris(2,2,3,3,3-pentafluoropropionylamide)
	N-(2-Chloro-4-{3-chloro-4-[(2,2,3,3,3-pentafluoropropanoyl)amino]benzyl}phenyl)-2,2,3,3,
Inchi:	InChI=1S/C22H9Cl2F15N2O3/c23-10-6-8(1-3-12(10)40-14(42)17(25,26)20(31,32)33)5-9
InchiKey:	SDEBSDSAEACUOY-UHFFFAOYSA-N
Formula:	C22H9Cl2F15N2O3
SMILES:	O=C(Nc1ccc(Cc2ccc(N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F)c(Cl)c2)cc1Cl)C(F)
Mol. weight [g/mol]:	705.20

Physical Properties

Property code	Value	Unit	Source
gf	-2794.90	kJ/mol	Joback Method
hf	-3312.60	kJ/mol	Joback Method
hfus	62.29	kJ/mol	Joback Method
hvap	89.22	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	7.975		Crippen Method
mcvol	349.020	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		NIST Webbook
tb	1044.79	K	Joback Method
tc	1284.68	K	Joback Method
tf	758.75	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.44	J/mol×K	1044.79	Joback Method
cpg	1099.13	J/mol×K	1084.77	Joback Method
cpg	1109.04	J/mol×K	1124.75	Joback Method

cpg	1119.47	J/mol×K	1164.74	Joback Method
cpg	1130.70	J/mol×K	1204.72	Joback Method
cpg	1143.04	J/mol×K	1244.70	Joback Method
cpg	1156.76	J/mol×K	1284.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373481&Units=SI

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