N,N'-(4-Chloro-1,2-phenylene)bis(2,2,3,3,3-pentafl

Inchi: InChI=1S/C12H5ClF10N2O2/c13-4-1-2-5(24-7(26)9(14,15)11(18,19)20)6(3-4)25-8(27)10
InchiKey: XLFNBCHMPWQPGF-UHFFFAOYSA-N
Formula: C12H5ClF10N2O2
SMILES: OC(=Nc1ccc(Cl)cc1N=C(O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 434.62

Physical Properties

Property code	Value	Unit	Source
hf	-2248.86	kJ/mol	Joback Method
hvap	77.08	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.911		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	1535.00		NIST Webbook
tb	865.29	K	Joback Method
tc	1061.89	K	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=U378220&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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