5-Chloro-2-methylaniline, N,N-bis(pentafluoropropionyl)-

Other names: N-(5-Chloro-2-methylphenyl)-N-(2,2,3,3,3-pentafluoropropanoyl)-2,2,3,3,3-pentafluoropro
Inchi: InChI=1S/C13H6ClF10NO2/c1-5-2-3-6(14)4-7(5)25(8(26)10(15,16)12(19,20)21)9(27)11(
InchiKey: DBEZOKYQVJEFTL-UHFFFAOYSA-N
Formula: C13H6ClF10NO2
SMILES: Cc1ccc(Cl)cc1N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 433.63

Physical Properties

Property code	Value	Unit	Source
gf	-1944.00	kJ/mol	Joback Method
hf	-2267.53	kJ/mol	Joback Method
hfus	34.25	kJ/mol	Joback Method
hvap	54.70	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.903		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	1183.00		NIST Webbook
rinpol	1183.00		NIST Webbook
tb	670.87	K	Joback Method
tc	847.81	K	Joback Method
tf	465.56	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.77	J/mol×K	670.87	Joback Method
cpg	601.66	J/mol×K	700.36	Joback Method
cpg	610.68	J/mol×K	729.85	Joback Method
cpg	618.92	J/mol×K	759.34	Joback Method
cpg	626.44	J/mol×K	788.83	Joback Method
cpg	633.33	J/mol×K	818.32	Joback Method
cpg	639.67	J/mol×K	847.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373248&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

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