5-Chloro-2-methyl-aniline, N,N-bis(heptafluorobutyryl)-

Inchi: InChI=1S/C15H6ClF14NO2/c1-5-2-3-6(16)4-7(5)31(8(32)10(17,18)12(21,22)14(25,26)27
InchiKey: XTWIKYIKGIIDHF-UHFFFAOYSA-N
Formula: C15H6ClF14NO2
SMILES: Cc1ccc(Cl)cc1N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 533.64

Physical Properties

Property code	Value	Unit	Source
gf	-2700.72	kJ/mol	Joback Method
hf	-3110.75	kJ/mol	Joback Method
hfus	36.92	kJ/mol	Joback Method
hvap	53.29	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.174		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	1232.00		NIST Webbook
tb	707.25	K	Joback Method
tc	877.02	K	Joback Method
tf	495.30	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.25	J/mol×K	707.25	Joback Method
cpg	740.82	J/mol×K	735.55	Joback Method
cpg	749.52	J/mol×K	763.84	Joback Method
cpg	757.45	J/mol×K	792.14	Joback Method
cpg	764.69	J/mol×K	820.43	Joback Method
cpg	771.34	J/mol×K	848.73	Joback Method
cpg	777.49	J/mol×K	877.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373250&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