5-Chloro-2-methyl-aniline, N-pentafluoropropionyl-

Inchi: InChI=1S/C10H7ClF5NO/c1-5-2-3-6(11)4-7(5)17-8(18)9(12,13)10(14,15)16/h2-4H,1H3,(
InchiKey: CYVMFAFINLFGOI-UHFFFAOYSA-N
Formula: C10H7ClF5NO
SMILES: Cc1ccc(Cl)cc1NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 287.61

Physical Properties

Property code	Value	Unit	Source
gf	-893.36	kJ/mol	Joback Method
hf	-1109.04	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	52.34	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.785		Crippen Method
mcvol	160.640	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1363.00		NIST Webbook
tb	596.20	K	Joback Method
tc	792.51	K	Joback Method
tf	394.22	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.51	J/mol×K	596.20	Joback Method
cpg	407.19	J/mol×K	628.92	Joback Method
cpg	417.04	J/mol×K	661.64	Joback Method
cpg	426.09	J/mol×K	694.36	Joback Method
cpg	434.43	J/mol×K	727.08	Joback Method
cpg	442.09	J/mol×K	759.79	Joback Method
cpg	449.13	J/mol×K	792.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373143&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