N-(2-Chloro-4-methylphenyl)-N-2,2,2-trifluoroacety

Inchi: InChI=1S/C11H6ClF6NO2/c1-5-2-3-7(6(12)4-5)19(8(20)10(13,14)15)9(21)11(16,17)18/h2
InchiKey: NDGNJHOCGPVVHN-UHFFFAOYSA-N
Formula: C11H6ClF6NO2
SMILES: Cc1ccc(N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)c(Cl)c1
Mol. weight [g/mol]: 333.61

Physical Properties

Property code	Value	Unit	Source
gf	-1187.28	kJ/mol	Joback Method
hf	-1424.31	kJ/mol	Joback Method
hfus	31.58	kJ/mol	Joback Method
hvap	56.11	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.633		Crippen Method
mcvol	178.070	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1231.00		NIST Webbook
rinpol	1231.00		NIST Webbook
tb	634.49	K	Joback Method
tc	824.55	K	Joback Method
tf	435.82	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.54	J/mol×K	634.49	Joback Method
cpg	464.60	J/mol×K	666.17	Joback Method
cpg	473.83	J/mol×K	697.84	Joback Method
cpg	482.31	J/mol×K	729.52	Joback Method
cpg	490.08	J/mol×K	761.20	Joback Method
cpg	497.20	J/mol×K	792.87	Joback Method
cpg	503.74	J/mol×K	824.55	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=U373205&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