N-(5-Chloro-2-methylphenyl)-2,2,2-trifluoroacetam

Inchi: InChI=1S/C9H7ClF3NO/c1-5-2-3-6(10)4-7(5)14-8(15)9(11,12)13/h2-4H,1H3,(H,14,15)
InchiKey: IASIUFGKIUHRAG-UHFFFAOYSA-N
Formula: C9H7ClF3NO
SMILES: Cc1ccc(Cl)cc1NC(=O)C(F)(F)F
Mol. weight [g/mol]: 237.61

Physical Properties

Property code	Value	Unit	Source
gf	-515.00	kJ/mol	Joback Method
hf	-687.43	kJ/mol	Joback Method
hfus	25.05	kJ/mol	Joback Method
hvap	53.05	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.149		Crippen Method
mcvol	143.010	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	578.01	K	Joback Method
tc	784.51	K	Joback Method
tf	379.35	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.31	J/mol×K	578.01	Joback Method
cpg	340.76	J/mol×K	612.43	Joback Method
cpg	350.45	J/mol×K	646.84	Joback Method
cpg	359.43	J/mol×K	681.26	Joback Method
cpg	367.73	J/mol×K	715.68	Joback Method
cpg	375.39	J/mol×K	750.10	Joback Method
cpg	382.46	J/mol×K	784.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373376&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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