N-Cyclohexyl-2,2,2-trifluoro-N-methylacetamide

Other names: Cyclohexanamine, N-methyl-, N-trifluoroacetyl-
N-Methyl-N-trifluoroacetyl-cyclohexanamine
Inchi: InChI=1S/C9H14F3NO/c1-13(8(14)9(10,11)12)7-5-3-2-4-6-7/h7H,2-6H2,1H3
InchiKey: YIPMXDYAKIORFF-UHFFFAOYSA-N
Formula: C9H14F3NO
SMILES: CN(C(=O)C(F)(F)F)C1CCCCC1
Mol. weight [g/mol]: 209.21

Physical Properties

Property code	Value	Unit	Source
gf	-550.38	kJ/mol	Joback Method
hf	-816.90	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	41.10	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.340		Crippen Method
mcvol	143.670	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1224.00		NIST Webbook
tb	485.76	K	Joback Method
tc	674.76	K	Joback Method
tf	285.16	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.13	J/mol×K	485.76	Joback Method
cpg	360.20	J/mol×K	517.26	Joback Method
cpg	376.23	J/mol×K	548.76	Joback Method
cpg	391.29	J/mol×K	580.26	Joback Method
cpg	405.41	J/mol×K	611.76	Joback Method
cpg	418.62	J/mol×K	643.26	Joback Method
cpg	430.98	J/mol×K	674.76	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=U373364&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