1-Chloro-1,1-difluoroacetylacetone

Inchi: InChI=1S/C5H5ClF2O2/c1-3(9)2-4(10)5(6,7)8/h2H2,1H3
InchiKey: ZPBKLXPYUKILDE-UHFFFAOYSA-N
Formula: C5H5ClF2O2
SMILES: CC(=O)CC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 170.54
CAS: 2375-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-665.33	kJ/mol	Joback Method
hf	-788.40	kJ/mol	Joback Method
hfus	14.85	kJ/mol	Joback Method
hvap	41.67	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.366		Crippen Method
mcvol	100.230	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
tb	454.28	K	Joback Method
tc	644.20	K	Joback Method
tf	279.49	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.23	J/mol×K	454.28	Joback Method
cpg	206.16	J/mol×K	485.93	Joback Method
cpg	213.57	J/mol×K	517.59	Joback Method
cpg	220.48	J/mol×K	549.24	Joback Method
cpg	226.93	J/mol×K	580.89	Joback Method
cpg	232.93	J/mol×K	612.55	Joback Method
cpg	238.51	J/mol×K	644.20	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=C2375760&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume