Methyl 2-chloro-2,2-difluoroacetate

Other names: Methyl chlorodifluoroacetate
Acetic acid, chlorodifluoro-, methyl ester
Inchi: InChI=1S/C3H3ClF2O2/c1-8-2(7)3(4,5)6/h1H3
InchiKey: AWUPLMYXZJKHEG-UHFFFAOYSA-N
Formula: C3H3ClF2O2
SMILES: COC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 144.50
CAS: 1514-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-658.25	kJ/mol	Joback Method
hf	-766.76	kJ/mol	Joback Method
hfus	9.26	kJ/mol	Joback Method
hvap	32.88	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.991		Crippen Method
mcvol	76.350	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	353.00	K	NIST Webbook
tc	557.15	K	Joback Method
tf	229.25	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.49	J/mol×K	377.07	Joback Method
cpg	142.32	J/mol×K	407.08	Joback Method
cpg	147.84	J/mol×K	437.10	Joback Method
cpg	153.06	J/mol×K	467.11	Joback Method
cpg	157.99	J/mol×K	497.12	Joback Method
cpg	162.64	J/mol×K	527.14	Joback Method
cpg	167.02	J/mol×K	557.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1514870&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume