1-chloro-1,1,3,3,3-pentafluoropropan-2-one

Inchi: InChI=1S/C3ClF5O/c4-2(5,6)1(10)3(7,8)9
InchiKey: OJUUDWYPNQALHZ-UHFFFAOYSA-N
Formula: C3ClF5O
SMILES: O=C(C(F)(F)F)C(F)(F)Cl
Mol. weight [g/mol]: 182.47

Physical Properties

Property code	Value	Unit	Source
gf	-1134.84	kJ/mol	Joback Method
hf	-1231.62	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	26.73	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.949		Crippen Method
mcvol	75.790	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	349.23	K	Joback Method
tc	510.94	K	Joback Method
tf	211.21	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.09	J/mol×K	349.23	Joback Method
cpg	149.68	J/mol×K	376.18	Joback Method
cpg	155.77	J/mol×K	403.13	Joback Method
cpg	161.38	J/mol×K	430.08	Joback Method
cpg	166.54	J/mol×K	457.04	Joback Method
cpg	171.27	J/mol×K	483.99	Joback Method
cpg	175.58	J/mol×K	510.94	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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1782.mol
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume