Chlorodifluoroacetamide

Other names: Difluorochloroacetamide
Acetamide, 2-chloro-2,2-difluoro-
2-chloro-2,2-difluoroacetamide
Inchi: InChI=1S/C2H2ClF2NO/c3-2(4,5)1(6)7/h(H2,6,7)
InchiKey: PSAKKOKLSDIKEK-UHFFFAOYSA-N
Formula: C2H2ClF2NO
SMILES: NC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 129.49
CAS: 354-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-495.22	kJ/mol	Joback Method
hf	-580.11	kJ/mol	Joback Method
hfus	10.67	kJ/mol	Joback Method
hvap	38.89	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.303		Crippen Method
mcvol	66.370	ml/mol	McGowan Method
pc	5116.65	kPa	Joback Method
tb	404.30	K	Joback Method
tc	601.82	K	Joback Method
tf	279.01	K	Joback Method
vc	0.257	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.07	J/mol×K	404.30	Joback Method
cpg	128.30	J/mol×K	437.22	Joback Method
cpg	133.11	J/mol×K	470.14	Joback Method
cpg	137.52	J/mol×K	503.06	Joback Method
cpg	141.55	J/mol×K	535.98	Joback Method
cpg	145.23	J/mol×K	568.90	Joback Method

cpg	148.58	J/mol×K	601.82	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=C354289&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