

Acetic acid, chlorodifluoro-

Other names:	Chlorodifluoroacetic acid
Inchi:	InChI=1S/C2HCIF2O2/c3-2(4,5)1(6)7/h(H,6,7)
InchiKey:	OAWAZQITIZDJRB-UHFFFAOYSA-N
Formula:	C2HCIF2O2
SMILES:	O=C(O)C(F)(F)Cl
Mol. weight [g/mol]:	130.48
CAS:	76-04-0

Physical Properties

Property code	Value	Unit	Source
gf	-698.49	kJ/mol	Joback Method
hf	-766.13	kJ/mol	Joback Method
hfus	9.57	kJ/mol	Joback Method
hvap	44.93	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	0.903		Crippen Method
mcvol	62.260	ml/mol	McGowan Method
pc	5382.80	kPa	Joback Method
tb	395.00	K	NIST Webbook
tb	395.20	K	NIST Webbook
tc	599.44	K	Joback Method
tf	256.57	K	Joback Method
vc	0.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.46	J/molxK	423.95	Joback Method
cpg	119.40	J/molxK	453.20	Joback Method
cpg	123.04	J/molxK	482.45	Joback Method
cpg	126.38	J/molxK	511.69	Joback Method
cpg	129.45	J/molxK	540.94	Joback Method
cpg	132.27	J/molxK	570.19	Joback Method
cpg	134.84	J/molxK	599.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76040&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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

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