Chlorodifluoroacetic anhydride

Other names: Acetic acid, chlorodifluoro-, anhydride
Inchi: InChI=1S/C4Cl2F4O3/c5-3(7,8)1(11)13-2(12)4(6,9)10
InchiKey: VBJIFLOSOQGDRZ-UHFFFAOYSA-N
Formula: C4Cl2F4O3
SMILES: O=C(OC(=O)C(F)(F)Cl)C(F)(F)Cl
Mol. weight [g/mol]: 242.94
CAS: 2834-23-3

Physical Properties

Property code	Value	Unit	Source
gf	-1177.46	kJ/mol	Joback Method
hf	-1316.69	kJ/mol	Joback Method
hfus	16.39	kJ/mol	Joback Method
hvap	43.31	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.719		Crippen Method
mcvol	107.790	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
tb	486.56	K	Joback Method
tc	675.64	K	Joback Method
tf	323.97	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.15	J/mol×K	486.56	Joback Method
cpg	227.17	J/mol×K	518.07	Joback Method
cpg	232.67	J/mol×K	549.59	Joback Method
cpg	237.67	J/mol×K	581.10	Joback Method
cpg	242.19	J/mol×K	612.61	Joback Method
cpg	246.27	J/mol×K	644.13	Joback Method
cpg	249.93	J/mol×K	675.64	Joback Method

Sources

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=C2834233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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