

2,2-Dichlorotrifluoroethyl chlorodifluoromethyl ether

Inchi: InChI=1S/C3Cl3F5O/c4-1(5,7)2(8,9)12-3(6,10)11
InchiKey: LWQARWCIQAGKRZ-UHFFFAOYSA-N
Formula: C3Cl3F5O
SMILES: FC(F)(Cl)OC(F)(F)C(F)(Cl)Cl
Mol. weight [g/mol]: 253.38
CAS: 37136-24-6

Physical Properties

Property code	Value	Unit	Source
chl	-787.40 ± 7.10	kJ/mol	NIST Webbook
gf	-1131.94	kJ/mol	Joback Method
hf	-1325.80 ± 7.30	kJ/mol	NIST Webbook
hfl	-1361.00 ± 7.10	kJ/mol	NIST Webbook
hfus	10.46	kJ/mol	Joback Method
hvap	33.80 ± 0.50	kJ/mol	NIST Webbook
log10ws	-3.69		Crippen Method
logp	3.486		Crippen Method
mcvol	104.570	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
tb	389.41	K	Joback Method
tc	565.83	K	Joback Method
tf	245.77	K	Joback Method
vc	0.425	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.85	J/mol×K	536.43	Joback Method
cpg	197.12	J/mol×K	389.41	Joback Method
cpg	204.33	J/mol×K	418.81	Joback Method
cpg	210.86	J/mol×K	448.22	Joback Method
cpg	216.77	J/mol×K	477.62	Joback Method
cpg	222.09	J/mol×K	507.02	Joback Method
cpg	231.09	J/mol×K	565.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37136246&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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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