

2,2-Dichlorotrifluoroethyl 1,1,3-trichlorotetrafluoropropyl ether

Inchi:	InChI=1S/C5Cl5F7O/c6-2(7,13)5(16,17)18-3(8,9)1(11,12)4(10,14)15
InchiKey:	CIARXPIAQOCSCO-UHFFFAOYSA-N
Formula:	C5Cl5F7O
SMILES:	FC(F)(Cl)C(F)(F)C(Cl)(Cl)OC(F)(F)C(F)(Cl)Cl
Mol. weight [g/mol]:	386.31
CAS:	61196-11-0

Physical Properties

Property code	Value	Unit	Source
chl	-1537.00 ± 4.60	kJ/mol	NIST Webbook
gf	-1522.90	kJ/mol	Joback Method
hf	-1752.50 ± 6.50	kJ/mol	NIST Webbook
hfl	-1805.00 ± 4.60	kJ/mol	NIST Webbook
hfus	15.37	kJ/mol	Joback Method
hvap	50.70 ± 0.80	kJ/mol	NIST Webbook
log10ws	-5.76		Crippen Method
logp	5.295		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
tb	502.11	K	Joback Method
tc	691.99	K	Joback Method
tf	334.17	K	Joback Method
vc	0.649	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.15	J/mol×K	502.11	Joback Method
cpg	349.27	J/mol×K	533.76	Joback Method
cpg	356.37	J/mol×K	565.40	Joback Method
cpg	362.52	J/mol×K	597.05	Joback Method
cpg	367.81	J/mol×K	628.70	Joback Method
cpg	372.32	J/mol×K	660.34	Joback Method
cpg	376.13	J/mol×K	691.99	Joback Method

Sources

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=C61196110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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