

Trichloro acetic acid, tripropylene glycol diester

Inchi:	InChI=1S/C13H18Cl6O6/c1-7(23-6-9(3)25-11(21)13(17,18)19)4-22-5-8(2)24-10(20)12(14)
InchiKey:	YPIYLWYEMBZFBP-UHFFFAOYSA-N
Formula:	C13H18Cl6O6
SMILES:	CC(COCC(C)OC(=O)C(Cl)(Cl)Cl)OCC(C)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	483.00

Physical Properties

Property code	Value	Unit	Source
gf	-692.48	kJ/mol	Joback Method
hf	-1193.47	kJ/mol	Joback Method
hfus	37.16	kJ/mol	Joback Method
hvap	90.22	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.012		Crippen Method
mcvol	294.090	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
tb	911.06	K	Joback Method
tc	1133.65	K	Joback Method
tf	564.41	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.10	J/mol×K	911.06	Joback Method
cpg	785.23	J/mol×K	948.16	Joback Method
cpg	793.30	J/mol×K	985.26	Joback Method
cpg	800.34	J/mol×K	1022.36	Joback Method
cpg	806.38	J/mol×K	1059.45	Joback Method
cpg	811.45	J/mol×K	1096.55	Joback Method
cpg	815.59	J/mol×K	1133.65	Joback Method
dvisc	0.0002253	Pa×s	564.41	Joback Method
dvisc	0.0001141	Pa×s	622.19	Joback Method
dvisc	0.0000648	Pa×s	679.96	Joback Method

dvisc	0.0000403	Pa×s	737.74	Joback Method
dvisc	0.0000268	Pa×s	795.51	Joback Method
dvisc	0.0000188	Pa×s	853.29	Joback Method
dvisc	0.0000138	Pa×s	911.06	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=B6001965&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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