2,2,2-Trichloroethanol, methyl ether

Inchi: InChI=1S/C3H5Cl3O/c1-7-2-3(4,5)6/h2H2,1H3
InchiKey: NZZHHOMCJICYCD-UHFFFAOYSA-N
Formula: C3H5Cl3O
SMILES: COCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 163.43

Physical Properties

Property code	Value	Unit	Source
gf	-163.57	kJ/mol	Joback Method
hf	-293.44	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	36.54	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	2.003		Crippen Method
mcvol	95.720	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	872.50		NIST Webbook
tb	399.52	K	Joback Method
tc	604.26	K	Joback Method
tf	237.98	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.06	J/mol×K	399.52	Joback Method
cpg	157.54	J/mol×K	433.64	Joback Method
cpg	163.61	J/mol×K	467.77	Joback Method
cpg	169.30	J/mol×K	501.89	Joback Method
cpg	174.62	J/mol×K	536.01	Joback Method
cpg	179.59	J/mol×K	570.13	Joback Method
cpg	184.23	J/mol×K	604.26	Joback Method
dvisc	0.0046556	Pa×s	237.98	Joback Method
dvisc	0.0024855	Pa×s	264.90	Joback Method

dvisc	0.0014899	Pa×s	291.83	Joback Method
dvisc	0.0009737	Pa×s	318.75	Joback Method
dvisc	0.0006800	Pa×s	345.67	Joback Method
dvisc	0.0005001	Pa×s	372.60	Joback Method
dvisc	0.0003834	Pa×s	399.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333841&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume