1,1,1-Trimethoxy-2-chloroethane

Inchi: InChI=1S/C5H11ClO3/c1-7-5(4-6,8-2)9-3/h4H2,1-3H3
InchiKey: NPEIUNVTLXEOLT-UHFFFAOYSA-N
Formula: C5H11ClO3
SMILES: COC(CCl)(OC)OC
Mol. weight [g/mol]: 154.59
CAS: 74974-54-2

Physical Properties

Property code	Value	Unit	Source
gf	-332.87	kJ/mol	Joback Method
hf	-614.00 ± 10.00	kJ/mol	NIST Webbook
hfl	-661.10 ± 8.80	kJ/mol	NIST Webbook
hfus	9.05	kJ/mol	Joback Method
hvap	47.50 ± 4.20	kJ/mol	NIST Webbook
log10ws	-0.43		Crippen Method
logp	0.818		Crippen Method
mcvol	111.160	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	415.26	K	Joback Method
tc	600.34	K	Joback Method
tf	245.14	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.40	J/mol×K	415.26	Joback Method
cpg	226.96	J/mol×K	446.11	Joback Method
cpg	236.22	J/mol×K	476.95	Joback Method
cpg	245.18	J/mol×K	507.80	Joback Method
cpg	253.83	J/mol×K	538.65	Joback Method
cpg	262.17	J/mol×K	569.50	Joback Method
cpg	270.20	J/mol×K	600.34	Joback Method
dvisc	0.0029645	Pa×s	245.14	Joback Method

dvisc	0.0015330	Pa×s	273.49	Joback Method
dvisc	0.0008973	Pa×s	301.85	Joback Method
dvisc	0.0005758	Pa×s	330.20	Joback Method
dvisc	0.0003964	Pa×s	358.55	Joback Method
dvisc	0.0002882	Pa×s	386.91	Joback Method
dvisc	0.0002189	Pa×s	415.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74974542&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
hfl:	Liquid phase 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