Propanoic acid, 2,2,3-trichloro-, methyl ester

Other names: Propionic acid, 2,2,3-trichloro-, methyl ester
Methyl 2,2,3-trichloropropanoate
Inchi: InChI=1S/C4H5Cl3O2/c1-9-3(8)4(6,7)2-5/h2H2,1H3
InchiKey: SXUZAHHOLLSZRC-UHFFFAOYSA-N
Formula: C4H5Cl3O2
SMILES: COC(=O)C(Cl)(Cl)CCl
Mol. weight [g/mol]: 191.44
CAS: 4749-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-284.07	kJ/mol	Joback Method
hf	-426.66	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	45.51	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.572		Crippen Method
mcvol	111.380	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	1031.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1031.00		NIST Webbook
tb	476.27	K	Joback Method
tc	690.53	K	Joback Method
tf	299.18	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.64	J/mol×K	476.27	Joback Method
cpg	202.69	J/mol×K	511.98	Joback Method

cpg	209.27	J/mol×K	547.69	Joback Method
cpg	215.39	J/mol×K	583.40	Joback Method
cpg	221.07	J/mol×K	619.11	Joback Method
cpg	226.33	J/mol×K	654.82	Joback Method
cpg	231.19	J/mol×K	690.53	Joback Method
dvisc	0.0033897	Pa×s	299.18	Joback Method
dvisc	0.0019690	Pa×s	328.69	Joback Method
dvisc	0.0012509	Pa×s	358.21	Joback Method
dvisc	0.0008515	Pa×s	387.73	Joback Method
dvisc	0.0006120	Pa×s	417.24	Joback Method
dvisc	0.0004595	Pa×s	446.75	Joback Method
dvisc	0.0003575	Pa×s	476.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4749353&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