Methyl-2,3,3,3-tetrachloropropanoate

Other names: Propanoic acid, 2,3,3,3-tetrachloro, methyl ester
Inchi: InChI=1S/C4H4Cl4O2/c1-10-3(9)2(5)4(6,7)8/h2H,1H3
InchiKey: LFHGTEYJIKRWFF-UHFFFAOYSA-N
Formula: C4H4Cl4O2
SMILES: COC(=O)C(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 225.88
CAS: 20618-10-4

Physical Properties

Property code	Value	Unit	Source
gf	-298.44	kJ/mol	Joback Method
hf	-447.68	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	49.51	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.137		Crippen Method
mcvol	123.620	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1137.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1137.00		NIST Webbook
tb	513.26	K	Joback Method
tc	738.13	K	Joback Method
tf	314.10	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.59	J/mol×K	513.26	Joback Method
cpg	243.95	J/mol×K	700.65	Joback Method
cpg	239.23	J/mol×K	663.17	Joback Method

cpg	234.07	J/mol×K	625.69	Joback Method
cpg	228.42	J/mol×K	588.22	Joback Method
cpg	222.27	J/mol×K	550.74	Joback Method
cpg	248.23	J/mol×K	738.13	Joback Method
dvisc	0.0003143	Pa×s	513.26	Joback Method
dvisc	0.0004125	Pa×s	480.07	Joback Method
dvisc	0.0005637	Pa×s	446.87	Joback Method
dvisc	0.0008101	Pa×s	413.68	Joback Method
dvisc	0.0012400	Pa×s	380.49	Joback Method
dvisc	0.0020592	Pa×s	347.29	Joback Method
dvisc	0.0038064	Pa×s	314.10	Joback Method

Sources

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=C20618104&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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