Methyl 3,3,3-trichloro-2-hydroxypropanoate

Inchi: InChI=1S/C4H5Cl3O3/c1-10-3(9)2(8)4(5,6)7/h2,8H,1H3
InchiKey: ZJUDLWOAOKTCQH-UHFFFAOYSA-N
Formula: C4H5Cl3O3
SMILES: COC(=O)C(O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 207.44

Physical Properties

Property code	Value	Unit	Source
gf	-423.33	kJ/mol	Joback Method
hf	-584.17	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	61.80	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	0.891		Crippen Method
mcvol	117.250	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	568.01	K	Joback Method
tc	772.13	K	Joback Method
tf	345.00	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.94	J/mol×K	568.01	Joback Method
cpg	235.89	J/mol×K	602.03	Joback Method
cpg	241.40	J/mol×K	636.05	Joback Method
cpg	246.51	J/mol×K	670.07	Joback Method
cpg	251.23	J/mol×K	704.09	Joback Method
cpg	255.58	J/mol×K	738.11	Joback Method
cpg	259.57	J/mol×K	772.13	Joback Method
dvisc	0.0068244	Pa×s	345.00	Joback Method
dvisc	0.0024965	Pa×s	382.17	Joback Method
dvisc	0.0010915	Pa×s	419.34	Joback Method

dvisc	0.0005460	Pa×s	456.50	Joback Method
dvisc	0.0003032	Pa×s	493.67	Joback Method
dvisc	0.0001828	Pa×s	530.84	Joback Method
dvisc	0.0001178	Pa×s	568.01	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=R80394&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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