METHYL 2,3,3-TRICHLOROPROPANOATE

Other names: Propanoic acid, 2,3,3-trichloro, methyl ester
Inchi: InChI=1S/C4H5Cl3O2/c1-9-4(8)2(5)3(6)7/h2-3H,1H3
InchiKey: VCJSVVVJNDJVPM-UHFFFAOYSA-N
Formula: C4H5Cl3O2
SMILES: COC(=O)C(Cl)C(Cl)Cl
Mol. weight [g/mol]: 191.44

Physical Properties

Property code	Value	Unit	Source
af	0.3708		Cheméo Relay (1.0)
hf	-507.07	kJ/mol	Cheméo Relay (1.0)
hfus	14.45	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Cheméo Relay (1.0)
ie	11.06	eV	Cheméo Relay (1.0)
log10ws	-1.65		Cheméo Relay (1.0)
logp	1.571		Crippen Method
mcvol	111.380	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	1031.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1029.00		NIST Webbook
tb	452.31	K	Cheméo Relay (1.0)
tc	672.96	K	Cheméo Relay (1.0)
tf	286.73	K	Cheméo Relay (1.0)
vc	0.385	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.56	J/mol×K	478.62	Joback Method
cpg	199.32	J/mol×K	513.66	Joback Method
cpg	205.76	J/mol×K	548.70	Joback Method

cpg	211.87	J/mol×K	583.74	Joback Method
cpg	217.64	J/mol×K	618.78	Joback Method
cpg	223.09	J/mol×K	653.82	Joback Method
cpg	228.21	J/mol×K	688.86	Joback Method
dvisc	0.0049718	Pa×s	266.76	Joback Method
dvisc	0.0024180	Pa×s	302.07	Joback Method
dvisc	0.0013676	Pa×s	337.38	Joback Method
dvisc	0.0008616	Pa×s	372.69	Joback Method
dvisc	0.0005881	Pa×s	408.00	Joback Method
dvisc	0.0004265	Pa×s	443.31	Joback Method
dvisc	0.0003244	Pa×s	478.62	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20618079&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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