

Methyl trichloropropenoate

Other names:	Methyl 2,3,3-trichloroacrylate 2,3,3-Trichloropropenoic acid, methyl ester Methyl 2,3,3-trichloropropenoate Acrylic acid, trichloro-, methyl ester Methyl trichloroacrylate
Inchi:	InChI=1S/C4H3Cl3O2/c1-9-4(8)2(5)3(6)7/h1H3
InchiKey:	LUAABZPMDXDUBN-UHFFFAOYSA-N
Formula:	C4H3Cl3O2
SMILES:	COC(=O)C(Cl)=C(Cl)Cl
Mol. weight [g/mol]:	189.42
CAS:	17640-12-9

Physical Properties

Property code	Value	Unit	Source
gf	-223.79	kJ/mol	Joback Method
hf	-320.27	kJ/mol	Joback Method
hfus	19.08	kJ/mol	Joback Method
hvap	46.93	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.045		Crippen Method
mcvol	107.080	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1022.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1484.00		NIST Webbook
tb	483.42	K	Joback Method
tc	702.50	K	Joback Method
tf	263.76	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.88	J/mol×K	483.42	Joback Method
cpg	179.60	J/mol×K	519.93	Joback Method
cpg	184.96	J/mol×K	556.45	Joback Method
cpg	189.97	J/mol×K	592.96	Joback Method
cpg	194.66	J/mol×K	629.47	Joback Method
cpg	199.02	J/mol×K	665.99	Joback Method
cpg	203.09	J/mol×K	702.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17640129&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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