

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

<b>Inchi:</b>	InChI=1S/C4H5Cl3O2/c1-9-3(8)2-4(5,6)7/h2H2,1H3
<b>InchiKey:</b>	FBMIRDYZKMXRFO-UHFFFAOYSA-N
<b>Formula:</b>	C4H5Cl3O2
<b>SMILES:</b>	COC(=O)CC(Cl)(Cl)Cl
<b>Mol. weight [g/mol]:</b>	191.44
<b>CAS:</b>	20618-02-4

## 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	-1.92		Crippen Method
logp	1.920		Crippen Method
mcvol	111.380	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	1017.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1018.00		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/molxK	476.27	Joback Method
cpg	202.69	J/molxK	511.98	Joback Method
cpg	209.27	J/molxK	547.69	Joback Method
cpg	215.39	J/molxK	583.40	Joback Method
cpg	221.07	J/molxK	619.11	Joback Method

cpg	226.33	J/molxK	654.82	Joback Method
cpg	231.19	J/molxK	690.53	Joback Method
dvisc	0.0033897	Paxs	299.18	Joback Method
dvisc	0.0019690	Paxs	328.69	Joback Method
dvisc	0.0012509	Paxs	358.21	Joback Method
dvisc	0.0008515	Paxs	387.73	Joback Method
dvisc	0.0006120	Paxs	417.24	Joback Method
dvisc	0.0004595	Paxs	446.75	Joback Method
dvisc	0.0003575	Paxs	476.27	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20618024&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20618024&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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