

Acetic acid, trichloro-, methyl ester

Other names:	Methyl trichloroacetate UN 2533
Inchi:	InChI=1S/C3H3Cl3O2/c1-8-2(7)3(4,5)6/h1H3
InchiKey:	VHFUHRXYRYWELT-UHFFFAOYSA-N
Formula:	C3H3Cl3O2
SMILES:	COC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	177.41
CAS:	598-99-2

Physical Properties

Property code	Value	Unit	Source
chl	-1211.00	kJ/mol	NIST Webbook
chl	-1218.00 ± 8.00	kJ/mol	NIST Webbook
gf	-292.49	kJ/mol	Joback Method
hf	-406.02	kJ/mol	Joback Method
hfus	11.49	kJ/mol	Joback Method
hvac	48.30 ± 0.10	kJ/mol	NIST Webbook
hvac	48.33 ± 0.12	kJ/mol	NIST Webbook
log10ws	-1.50		Crippen Method
logp	1.530		Crippen Method
mccol	97.290	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
ripol	867.00		NIST Webbook
ripol	875.00		NIST Webbook
ripol	895.50		NIST Webbook
ripol	934.00		NIST Webbook
ripol	896.00		NIST Webbook
ripol	902.00		NIST Webbook
ripol	875.00		NIST Webbook
ripol	897.00		NIST Webbook
ripol	896.00		NIST Webbook
ripol	912.00		NIST Webbook
ripol	884.00		NIST Webbook
ripol	876.00		NIST Webbook
ripol	896.00		NIST Webbook
ripol	897.00		NIST Webbook
ripol	1387.00		NIST Webbook

ripol	1392.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1387.00		NIST Webbook
tb	425.70	K	NIST Webbook
tb	427.00	K	NIST Webbook
tb	427.00 ± 3.00	K	NIST Webbook
tb	427.00 ± 0.20	K	NIST Webbook
tc	670.81	K	Joback Method
tf	255.70 ± 0.40	K	NIST Webbook
vc	0.363	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.77	J/molxK	453.39	Joback Method
cpg	182.89	J/molxK	634.58	Joback Method
cpg	178.81	J/molxK	598.34	Joback Method
cpg	174.38	J/molxK	562.10	Joback Method
cpg	169.57	J/molxK	525.86	Joback Method
cpg	164.37	J/molxK	489.63	Joback Method
cpg	186.63	J/molxK	670.81	Joback Method
dvisc	0.0003979	Paxs	453.39	Joback Method
dvisc	0.0005084	Paxs	425.81	Joback Method
dvisc	0.0006720	Paxs	398.23	Joback Method
dvisc	0.0009260	Paxs	370.65	Joback Method
dvisc	0.0013435	Paxs	343.07	Joback Method
dvisc	0.0020802	Paxs	315.49	Joback Method
dvisc	0.0035022	Paxs	287.91	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=C598992&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

chl:	Standard liquid enthalpy of combustion
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
mccvol:	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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