Acetic acid, dichloro-, methyl ester

Other names: Dichloroacetic acid methyl ester
Methyl dichloroacetate
UN 2299
Inchi: InChI=1S/C3H4Cl2O2/c1-7-3(6)2(4)5/h2H,1H3
InchiKey: HKMLRUAPIDAGIE-UHFFFAOYSA-N
Formula: C3H4Cl2O2
SMILES: COC(=O)C(Cl)Cl
Mol. weight [g/mol]: 142.97
CAS: 116-54-1

Physical Properties

Property code	Value	Unit	Source
chl	-1312.00	kJ/mol	NIST Webbook
chl	-1316.00 ± 4.00	kJ/mol	NIST Webbook
gf	-285.84	kJ/mol	Joback Method
hf	-386.81	kJ/mol	Joback Method
hfus	11.18	kJ/mol	Joback Method
hvap	38.00	kJ/mol	NIST Webbook
hvap	47.70 ± 0.10	kJ/mol	NIST Webbook
hvap	47.72 ± 0.10	kJ/mol	NIST Webbook
log10ws	-0.85		Crippen Method
logp	0.963		Crippen Method
mcvol	85.050	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
rinpol	792.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	811.50		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	792.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1365.00		NIST Webbook

ripol	1387.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1391.00		NIST Webbook
tb	416.00 ± 3.00	K	NIST Webbook
tb	416.00	K	NIST Webbook
tc	620.11	K	Joback Method
tf	221.20 ± 0.02	K	NIST Webbook
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.59	J/mol×K	586.55	Joback Method
cpg	157.07	J/mol×K	552.99	Joback Method
cpg	152.35	J/mol×K	519.43	Joback Method
cpg	147.43	J/mol×K	485.87	Joback Method
cpg	142.32	J/mol×K	452.31	Joback Method
cpg	137.02	J/mol×K	418.75	Joback Method
cpg	165.90	J/mol×K	620.11	Joback Method
dvisc	0.0038551	Pa×s	240.57	Joback Method
dvisc	0.0003593	Pa×s	418.75	Joback Method
dvisc	0.0004588	Pa×s	389.05	Joback Method
dvisc	0.0006101	Pa×s	359.36	Joback Method
dvisc	0.0008540	Pa×s	329.66	Joback Method
dvisc	0.0012778	Pa×s	299.96	Joback Method
dvisc	0.0020888	Pa×s	270.27	Joback Method
hvapt	44.90	kJ/mol	406.00	NIST Webbook
hvapt	47.20	kJ/mol	346.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47756e+01
Coeff. B	-3.57133e+03
Coeff. C	-6.44470e+01

Temperature range (K), min.	310.95
Temperature range (K), max.	441.80

Sources

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=C116541&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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