

Acetic acid, hydroxy-, methyl ester

Other names:	Methyl ester of hydroxyacetic acid glycolic acid, methyl ester methyl glycolate methyl hydroxyacetate methyl hydroxyethanoate
Inchi:	InChI=1S/C3H6O3/c1-6-3(5)2-4/h4H,2H2,1H3
InchiKey:	GSJFXBNYJCXDGI-UHFFFAOYSA-N
Formula:	C3H6O3
SMILES:	COC(=O)CO
Mol. weight [g/mol]:	90.08
CAS:	96-35-5

Physical Properties

Property code	Value	Unit	Source
chl	-1428.61 ± 0.94	kJ/mol	NIST Webbook
gf	-396.36	kJ/mol	Joback Method
hf	-556.90 ± 6.40	kJ/mol	NIST Webbook
hfl	-609.41 ± 0.94	kJ/mol	NIST Webbook
hfus	10.40	kJ/mol	Joback Method
hvap	52.50 ± 6.30	kJ/mol	NIST Webbook
hvap	52.50	kJ/mol	NIST Webbook
hvap	52.50 ± 6.30	kJ/mol	NIST Webbook
ie	10.42 ± 0.05	eV	NIST Webbook
log10ws	0.80		Crippen Method
logp	-0.848		Crippen Method
mcvol	66.440	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
ripol	1403.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1403.00		NIST Webbook
tb	423.20	K	NIST Webbook
tc	611.34	K	Joback Method
tf	256.55	K	Joback Method
vc	0.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.32	J/mol×K	436.51	Joback Method
cpg	158.17	J/mol×K	611.34	Joback Method
cpg	153.74	J/mol×K	582.20	Joback Method
cpg	149.15	J/mol×K	553.06	Joback Method
cpg	144.41	J/mol×K	523.92	Joback Method
cpg	139.52	J/mol×K	494.79	Joback Method
cpg	134.49	J/mol×K	465.65	Joback Method
dvisc	0.0063665	Pa×s	286.54	Joback Method
dvisc	0.0026236	Pa×s	316.54	Joback Method
dvisc	0.0012605	Pa×s	346.53	Joback Method
dvisc	0.0006806	Pa×s	376.52	Joback Method
dvisc	0.0004025	Pa×s	406.52	Joback Method
dvisc	0.0002559	Pa×s	436.51	Joback Method
dvisc	0.0190072	Pa×s	256.55	Joback Method
hfust	11.40	kJ/mol	272.80	NIST Webbook
hvapt	47.40	kJ/mol	353.50	NIST Webbook
pvap	9.29	kPa	353.25	Binary vapor liquid equilibrium of methyl glycolate and ethylene glycol
pvap	5.91	kPa	343.26	Binary vapor liquid equilibrium of methyl glycolate and ethylene glycol
pvap	3.74	kPa	333.28	Binary vapor liquid equilibrium of methyl glycolate and ethylene glycol
pvap	2.31	kPa	323.12	Binary vapor liquid equilibrium of methyl glycolate and ethylene glycol
pvap	1.41	kPa	313.27	Binary vapor liquid equilibrium of methyl glycolate and ethylene glycol
pvap	0.85	kPa	303.17	Binary vapor liquid equilibrium of methyl glycolate and ethylene glycol

pvap	0.49	kPa	293.23	Binary vapor liquid equilibrium of methyl glycolate and ethylene glycol
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Binary vapor liquid equilibrium of methyl glycolate and ethylene glycol:	https://www.doi.org/10.1016/j.fluid.2006.09.019
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=C96355&Units=SI

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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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