

Acetic acid, hydroxy-, propyl ester

Other names:	Propyl glycolate Glycolic acid, propyl ester Hydroxyacetic acid propyl ester
Inchi:	InChI=1S/C5H10O3/c1-2-3-8-5(7)4-6/h6H,2-4H2,1H3
InchiKey:	NORCOOJYTVHQCR-UHFFFAOYSA-N
Formula:	C5H10O3
SMILES:	CCCOC(=O)CO
Mol. weight [g/mol]:	118.13
CAS:	90357-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-379.52	kJ/mol	Joback Method
hf	-543.56	kJ/mol	Joback Method
hfus	15.58	kJ/mol	Joback Method
hvap	52.56	kJ/mol	Joback Method
log10ws	-0.04		Crippen Method
logp	-0.068		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	482.27	K	Joback Method
tc	654.52	K	Joback Method
tf	279.09	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.55	J/mol×K	482.27	Joback Method
cpg	212.29	J/mol×K	510.98	Joback Method
cpg	219.76	J/mol×K	539.69	Joback Method
cpg	226.98	J/mol×K	568.39	Joback Method
cpg	233.93	J/mol×K	597.10	Joback Method
cpg	240.63	J/mol×K	625.81	Joback Method

cpg	247.05	J/mol×K	654.52	Joback Method
dvisc	0.0141369	Pa×s	279.09	Joback Method
dvisc	0.0046479	Pa×s	312.95	Joback Method
dvisc	0.0018989	Pa×s	346.82	Joback Method
dvisc	0.0009097	Pa×s	380.68	Joback Method
dvisc	0.0004915	Pa×s	414.54	Joback Method
dvisc	0.0002914	Pa×s	448.41	Joback Method
dvisc	0.0001860	Pa×s	482.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90357587&Units=SI

Legend

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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