

Acetic acid, 3-hydroxypropyl ester

Inchi:	InChI=1S/C5H10O3/c1-5(7)8-4-2-3-6/h6H,2-4H2,1H3
InchiKey:	DOUBAFNWWVFAWEC-UHFFFAOYSA-N
Formula:	C5H10O3
SMILES:	CC(=O)OCCCO
Mol. weight [g/mol]:	118.13

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
ripol	947.00		NIST Webbook
ripol	1754.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1754.00		NIST Webbook
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/molxK	482.27	Joback Method
cpg	212.29	J/molxK	510.98	Joback Method
cpg	219.76	J/molxK	539.69	Joback Method
cpg	226.98	J/molxK	568.39	Joback Method
cpg	233.93	J/molxK	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	Paxs	279.09	Joback Method
dvisc	0.0046479	Paxs	312.95	Joback Method
dvisc	0.0018989	Paxs	346.82	Joback Method
dvisc	0.0009097	Paxs	380.68	Joback Method
dvisc	0.0004915	Paxs	414.54	Joback Method
dvisc	0.0002914	Paxs	448.41	Joback Method
dvisc	0.0001860	Paxs	482.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R323032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
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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