

Propyl butanoate, 3-hydroxy

Inchi:	InChI=1S/C7H14O3/c1-3-4-10-7(9)5-6(2)8/h6,8H,3-5H2,1-2H3
InchiKey:	DYIMQAHDHMHISM-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	CCCOC(=O)CC(C)O
Mol. weight [g/mol]:	146.18

Physical Properties

Property code	Value	Unit	Source
gf	-365.12	kJ/mol	Joback Method
hf	-590.12	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	56.62	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.710		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	980.00		NIST Webbook
rinpol	979.00		NIST Webbook
tb	527.59	K	Joback Method
tc	700.51	K	Joback Method
tf	286.63	K	Joback Method
vc	0.465	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.76	J/molxK	527.59	Joback Method
cpg	298.85	J/molxK	556.41	Joback Method
cpg	308.56	J/molxK	585.23	Joback Method
cpg	317.88	J/molxK	614.05	Joback Method
cpg	326.83	J/molxK	642.87	Joback Method
cpg	335.40	J/molxK	671.69	Joback Method
cpg	343.59	J/molxK	700.51	Joback Method
dvisc	0.0172601	Paxs	286.63	Joback Method

dvisc	0.0045782	Paxs	326.79	Joback Method
dvisc	0.0016237	Paxs	366.95	Joback Method
dvisc	0.0007065	Paxs	407.11	Joback Method
dvisc	0.0003570	Paxs	447.27	Joback Method
dvisc	0.0002019	Paxs	487.43	Joback Method
dvisc	0.0001245	Paxs	527.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R59880&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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