

Propyl 3-hydroxybutanoate

Inchi:	InChI=1S/C6H12O3/c1-2-6(8)9-5-3-4-7/h7H,2-5H2,1H3
InchiKey:	AYIRHANHVDOYDJ-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	CCC(=O)OCCCO
Mol. weight [g/mol]:	132.16

Physical Properties

Property code	Value	Unit	Source
gf	-371.10	kJ/mol	Joback Method
hf	-564.20	kJ/mol	Joback Method
hfus	18.17	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	0.322		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	972.00		NIST Webbook
rinpol	972.00		NIST Webbook
tb	505.15	K	Joback Method
tc	676.09	K	Joback Method
tf	290.36	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.47	J/molxK	505.15	Joback Method
cpg	254.32	J/molxK	533.64	Joback Method
cpg	262.85	J/molxK	562.13	Joback Method
cpg	271.06	J/molxK	590.62	Joback Method
cpg	278.97	J/molxK	619.11	Joback Method
cpg	286.56	J/molxK	647.60	Joback Method
cpg	293.84	J/molxK	676.09	Joback Method
dvisc	0.0120283	Paxs	290.36	Joback Method

dvisc	0.0039241	Paxs	326.16	Joback Method
dvisc	0.0015977	Paxs	361.96	Joback Method
dvisc	0.0007647	Paxs	397.75	Joback Method
dvisc	0.0004134	Paxs	433.55	Joback Method
dvisc	0.0002454	Paxs	469.35	Joback Method
dvisc	0.0001569	Paxs	505.15	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=R66988&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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