Butanoic acid, 2,3-dihydroxypropyl ester

Other names:	«alpha»-Monobutyrin
	Butyrin, 1-mono-
	Glycerol-«alpha»-mono-n-butyrate
	1-Monobutyrin
	Mono-n-butyrin
	1-Mono-n-butyrin
	2,3-dihydroxypropyl butyrate
	(dl) butyric acid, 2,3-dihydroxypropyl ester
Inchi:	InChI=1S/C7H14O4/c1-2-3-7(10)11-5-6(9)4-8/h6,8-9H,2-5H2,1H3
InchiKey:	RIEABXYBQSLTFR-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	CCCC(=O)OCC(O)CO
Mol. weight [g/mol]:	146.18
CAS:	557-25-5

Physical Properties

Property code	Value	Unit	Source
gf	-501.94	kJ/mol	Joback Method
hf	-742.35	kJ/mol	Joback Method
hfus	21.33	kJ/mol	Joback Method
hvap	73.30	kJ/mol	Joback Method
log10ws	-0.25		Crippen Method
logp	-0.317		Crippen Method
mcvol	128.670	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	619.77	K	Joback Method
tc	787.77	K	Joback Method
tf	347.45	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.13	J/mol×K	787.77	Joback Method

cpg	336.70	J/mol×K	619.77	Joback Method
cpg	345.52	J/mol×K	647.77	Joback Method
cpg	353.98	J/mol×K	675.77	Joback Method
cpg	362.06	J/mol×K	703.77	Joback Method
cpg	369.78	J/mol×K	731.77	Joback Method
cpg	377.14	J/mol×K	759.77	Joback Method
dvisc	0.0000269	Pa×s	619.77	Joback Method
dvisc	0.0118715	Pa×s	347.45	Joback Method
dvisc	0.0023943	Pa×s	392.84	Joback Method
dvisc	0.0006728	Pa×s	438.22	Joback Method
dvisc	0.0002399	Pa×s	483.61	Joback Method
dvisc	0.0001021	Pa×s	529.00	Joback Method
dvisc	0.0000497	Pa×s	574.38	Joback Method
hvapt	80.40	kJ/mol	420.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C557255&Units=SI
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

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
hvapt:	Enthalpy of vaporization at a given temperature
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