Butanoic acid, 3-hydroxy-, butyl ester

Other names:	Butyl 3-hydroxybutyrate
	Butyl 3-hydroxybutanoate
Inchi:	InChI=1S/C8H16O3/c1-3-4-5-11-8(10)6-7(2)9/h7,9H,3-6H2,1-2H3
InchiKey:	LHDWRKCOQQHAMP-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCCCOC(=O)CC(C)O
Mol. weight [g/mol]:	160.21
CAS:	53605-94-0

Physical Properties

Property code	Value	Unit	Source
gf	-356.70	kJ/mol	Joback Method
hf	-610.76	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.101		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1111.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1707.00		NIST Webbook
tb	550.47	K	Joback Method
tc	722.09	K	Joback Method
tf	297.90	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.69	J/mol×K	550.47	Joback Method
cpg	344.69	J/mol×K	579.07	Joback Method
cpg	355.26	J/mol×K	607.68	Joback Method
cpg	365.40	J/mol×K	636.28	Joback Method
cpg	375.11	J/mol×K	664.88	Joback Method
cpg	384.41	J/mol×K	693.49	Joback Method
cpg	393.29	J/mol×K	722.09	Joback Method
dvisc	0.0141338	Pa×s	297.90	Joback Method
dvisc	0.0037547	Pa×s	340.00	Joback Method
dvisc	0.0013358	Pa×s	382.09	Joback Method
dvisc	0.0005834	Pa×s	424.19	Joback Method
dvisc	0.0002959	Pa×s	466.28	Joback Method
dvisc	0.0001680	Pa×s	508.38	Joback Method
dvisc	0.0001040	Pa×s	550.47	Joback Method

Sources

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=C53605940&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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