Butanoic acid, 1-methylpropyl ester

Other names:	Butyric acid, sec-butyl ester
	sec-Butyl Butyrate
	Butanoic acid, 2-butyl ester
Inchi:	InChI=1S/C8H16O2/c1-4-6-8(9)10-7(3)5-2/h7H,4-6H2,1-3H3
InchiKey:	QJHDFBAAFGELLO-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCC(=O)OC(C)CC
Mol. weight [g/mol]:	144.21
CAS:	819-97-6

Physical Properties

Property code	Value	Unit	Source
chl	-4842.10 ± 3.80	kJ/mol	NIST Webbook
gf	-219.88	kJ/mol	Joback Method
hf	-545.20 ± 4.20	kJ/mol	NIST Webbook
hfl	-592.00 ± 4.00	kJ/mol	NIST Webbook
hfus	15.74	kJ/mol	Joback Method
hvap	47.00 ± 1.00	kJ/mol	NIST Webbook
hvap	46.80	kJ/mol	NIST Webbook
log10ws	-2.15		Crippen Method
logp	2.128		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	925.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	906.00		NIST Webbook
ripol	1159.00		NIST Webbook

ripol	1140.00		NIST Webbook
ripol	1140.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1144.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1138.00		NIST Webbook
ripol	1158.00		NIST Webbook
ripol	1200.00		NIST Webbook
tb	424.65 ± 1.00	K	NIST Webbook
tc	637.16	K	Joback Method
tf	237.08	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	338.23	J/mol×K	607.34	Joback Method
cpg	348.57	J/mol×K	637.16	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
dvisc	0.0002420	Pa×s	458.29	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=C819976&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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