Butanoic acid, 1,2-dimethylpropyl ester

Inchi: InChI=1S/C9H18O2/c1-5-6-9(10)11-8(4)7(2)3/h7-8H,5-6H2,1-4H3
InchiKey: YBSMWGNIGFSKPE-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 158.24

Physical Properties

Property code	Value	Unit	Source
gf	-213.90	kJ/mol	Joback Method
hf	-484.45	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.374		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	993.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1210.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1243.00		NIST Webbook
tb	480.73	K	Joback Method
tc	661.81	K	Joback Method
tf	233.35	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.22	J/mol×K	480.73	Joback Method
cpg	337.19	J/mol×K	510.91	Joback Method
cpg	350.61	J/mol×K	541.09	Joback Method
cpg	363.51	J/mol×K	571.27	Joback Method
cpg	375.88	J/mol×K	601.45	Joback Method
cpg	387.73	J/mol×K	631.63	Joback Method
cpg	399.06	J/mol×K	661.81	Joback Method
dvisc	0.0073761	Pa×s	233.35	Joback Method
dvisc	0.0026314	Pa×s	274.58	Joback Method
dvisc	0.0012286	Pa×s	315.81	Joback Method
dvisc	0.0006840	Pa×s	357.04	Joback Method
dvisc	0.0004299	Pa×s	398.27	Joback Method
dvisc	0.0002948	Pa×s	439.50	Joback Method
dvisc	0.0002156	Pa×s	480.73	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28522&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume