Butanoic acid, 1,1-dimethylethyl ester

Other names: CH3CH2CH2C(O)OC(CH3)3
tert-Butyl butyrate
Inchi: InChI=1S/C8H16O2/c1-5-6-7(9)10-8(2,3)4/h5-6H2,1-4H3
InchiKey: TWBUVVYSQBFVGZ-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCCC(=O)OC(C)(C)C
Mol. weight [g/mol]: 144.21
CAS: 2308-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-214.60	kJ/mol	Joback Method
hf	-462.00	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	41.26	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.128		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	873.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	862.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1090.00		NIST Webbook
tb	409.40 ± 2.00	K	NIST Webbook
tc	641.54	K	Joback Method
tf	254.50	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.32	J/mol×K	455.50	Joback Method
cpg	295.73	J/mol×K	486.51	Joback Method
cpg	308.53	J/mol×K	517.51	Joback Method
cpg	320.73	J/mol×K	548.52	Joback Method
cpg	332.35	J/mol×K	579.53	Joback Method
cpg	343.41	J/mol×K	610.54	Joback Method
cpg	353.92	J/mol×K	641.54	Joback Method
dvisc	0.0046923	Pa×s	254.50	Joback Method
dvisc	0.0021847	Pa×s	288.00	Joback Method
dvisc	0.0011929	Pa×s	321.50	Joback Method
dvisc	0.0007301	Pa×s	355.00	Joback Method
dvisc	0.0004864	Pa×s	388.50	Joback Method
dvisc	0.0003456	Pa×s	422.00	Joback Method
dvisc	0.0002582	Pa×s	455.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2308385&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
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