Butanoic acid, 1,1-dimethyl-2-phenylethyl ester

Other names: Butyric acid, «alpha»,«alpha»-dimethylphenethyl ester
«alpha»,«alpha»-Dimethylphenethyl alcohol, butyrate
«alpha»,«alpha»-Dimethylphenethyl butyrate
Benzyl dimethylcarbinyl butyrate
Benzyl dimethylcarbinyl n-butyrate
Dimethylbenzylcarbinyl butyrate
Dimethyl benzyl carbinyl n-butyrate
1,1-Dimethyl-2-phenylethyl butyrate

Inchi: InChI=1S/C14H20O2/c1-4-8-13(15)16-14(2,3)11-12-9-6-5-7-10-12/h5-7,9-10H,4,8,11H2,

InchiKey: SHSGYHAHMQLYRB-UHFFFAOYSA-N

Formula: C14H20O2

SMILES: CCCC(=O)OC(C)(C)Cc1ccccc1

Mol. weight [g/mol]: 220.31

CAS: 10094-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-51.67	kJ/mol	Joback Method
hf	-349.31	kJ/mol	Joback Method
hfus	21.43	kJ/mol	Joback Method
hvap	56.89	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.351		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1488.00		NIST Webbook
rinpol	1476.00		NIST Webbook
ripol	1889.00		NIST Webbook
tb	619.46	K	Joback Method
tc	830.73	K	Joback Method
tf	348.54	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.15	J/mol×K	619.46	Joback Method
cpg	514.27	J/mol×K	654.67	Joback Method
cpg	530.30	J/mol×K	689.88	Joback Method
cpg	545.29	J/mol×K	725.10	Joback Method
cpg	559.29	J/mol×K	760.31	Joback Method
cpg	572.34	J/mol×K	795.52	Joback Method
cpg	584.50	J/mol×K	830.73	Joback Method
dvisc	0.0023056	Pa×s	348.54	Joback Method
dvisc	0.0010920	Pa×s	393.69	Joback Method
dvisc	0.0006032	Pa×s	438.85	Joback Method
dvisc	0.0003722	Pa×s	484.00	Joback Method
dvisc	0.0002494	Pa×s	529.15	Joback Method
dvisc	0.0001780	Pa×s	574.31	Joback Method
dvisc	0.0001334	Pa×s	619.46	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=C10094345&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