BUTANOIC ACID, 2-HYDROXY-2-METHYL-, METHYL ESTER

Other names: methyl 2-hydroxy-2-methylbutanoate
Inchi: InChI=1S/C6H12O3/c1-4-6(2,8)5(7)9-3/h8H,4H2,1-3H3
InchiKey: FMXYCZVOMYLMKM-UHFFFAOYSA-N
Formula: C6H12O3
SMILES: CCC(C)(O)C(=O)OC
Mol. weight [g/mol]: 132.16

Physical Properties

Property code	Value	Unit	Source
hf	-657.00	kJ/mol	Cheméo Relay (1.0)
hfus	10.76	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Cheméo Relay (1.0)
ie	10.08	eV	Cheméo Relay (1.0)
logp	0.320		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
rinpol	923.00		NIST Webbook
ripol	1272.00		NIST Webbook
ripol	1281.00		NIST Webbook
tb	430.60	K	Cheméo Relay (1.0)
tf	248.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.95	J/mol×K	501.92	Joback Method
cpg	258.51	J/mol×K	532.05	Joback Method
cpg	267.61	J/mol×K	562.19	Joback Method
cpg	276.27	J/mol×K	592.32	Joback Method
cpg	284.51	J/mol×K	622.45	Joback Method
cpg	292.32	J/mol×K	652.58	Joback Method
cpg	299.73	J/mol×K	682.72	Joback Method
dvisc	0.0147388	Pa×s	292.78	Joback Method
dvisc	0.0046012	Pa×s	327.64	Joback Method
dvisc	0.0017968	Pa×s	362.49	Joback Method

dvisc	0.0008275	Pa×s	397.35	Joback Method
dvisc	0.0004319	Pa×s	432.21	Joback Method
dvisc	0.0002484	Pa×s	467.06	Joback Method
dvisc	0.0001543	Pa×s	501.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32793343&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point