Butanedioic acid, 2-hydroxy-2-(1-methylethyl), dimethyl ester

Other names: 2-Hydroxy-2-isopropyl-succinic acid dimethyl ester
dimethyl 2-hydroxy-2-(isopropyl)succinate
Inchi: InChI=1S/C9H16O5/c1-6(2)9(12,8(11)14-4)5-7(10)13-3/h6,12H,5H2,1-4H3
InchiKey: OQIDMHZJNDYZLB-UHFFFAOYSA-N
Formula: C9H16O5
SMILES: COC(=O)CC(O)(C(=O)OC)C(C)C
Mol. weight [g/mol]: 204.22
CAS: 43064-52-4

Physical Properties

Property code	Value	Unit	Source
gf	-579.36	kJ/mol	Joback Method
hf	-884.95	kJ/mol	Joback Method
hfus	17.79	kJ/mol	Joback Method
hvap	68.93	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.110		Crippen Method
mcvol	158.420	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	1247.00		NIST Webbook
rinpol	1247.00		NIST Webbook
tb	646.41	K	Joback Method
tc	832.31	K	Joback Method
tf	383.75	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.23	J/mol×K	646.41	Joback Method
cpg	436.45	J/mol×K	677.39	Joback Method
cpg	447.07	J/mol×K	708.38	Joback Method
cpg	457.10	J/mol×K	739.36	Joback Method
cpg	466.55	J/mol×K	770.34	Joback Method

cpg	475.42	J/mol×K	801.33	Joback Method
cpg	483.74	J/mol×K	832.31	Joback Method
dvisc	0.0028806	Pa×s	383.75	Joback Method
dvisc	0.0010196	Pa×s	427.53	Joback Method
dvisc	0.0004377	Pa×s	471.30	Joback Method
dvisc	0.0002169	Pa×s	515.08	Joback Method
dvisc	0.0001200	Pa×s	558.86	Joback Method
dvisc	0.0000724	Pa×s	602.63	Joback Method
dvisc	0.0000467	Pa×s	646.41	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=C43064524&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume