Butanedioic acid, 2-butyl-2-hydroxy, dimethyl ester

Inchi: InChI=1S/C10H18O5/c1-4-5-6-10(13,9(12)15-3)7-8(11)14-2/h13H,4-7H2,1-3H3
InchiKey: UKPAYNWDOKISQR-UHFFFAOYSA-N
Formula: C10H18O5
SMILES: CCCCC(O)(CC(=O)OC)C(=O)OC
Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
gf	-568.50	kJ/mol	Joback Method
hf	-900.31	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	71.55	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	0.644		Crippen Method
mcvol	172.510	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	1341.00		NIST Webbook
tb	669.73	K	Joback Method
tc	851.57	K	Joback Method
tf	410.02	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.92	J/mol×K	669.73	Joback Method
cpg	486.56	J/mol×K	700.04	Joback Method
cpg	497.59	J/mol×K	730.34	Joback Method
cpg	508.02	J/mol×K	760.65	Joback Method
cpg	517.85	J/mol×K	790.96	Joback Method
cpg	527.11	J/mol×K	821.27	Joback Method
cpg	535.79	J/mol×K	851.57	Joback Method
dvisc	0.0017280	Pa×s	410.02	Joback Method
dvisc	0.0006889	Pa×s	453.31	Joback Method

dvisc	0.0003224	Pa×s	496.59	Joback Method
dvisc	0.0001704	Pa×s	539.88	Joback Method
dvisc	0.0000990	Pa×s	583.16	Joback Method
dvisc	0.0000620	Pa×s	626.44	Joback Method
dvisc	0.0000413	Pa×s	669.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R106486&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

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