Pentanedioic acid, 3-hydroxy-3-(1-methylethyl), dimethyl ester

Inchi: InChI=1S/C10H18O5/c1-7(2)10(13,5-8(11)14-3)6-9(12)15-4/h7,13H,5-6H2,1-4H3

InchiKey: IBYRCUNEKPBGQF-UHFFFAOYSA-N

Formula: C10H18O5

SMILES: COC(=O)CC(O)(CC(=O)OC)C(C)C

Mol. weight [g/mol]: 218.25

Physical Properties

Property code	Value	Unit	Source
gf	-570.94	kJ/mol	Joback Method
hf	-905.59	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.500		Crippen Method
mcvol	172.510	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	669.29	K	Joback Method
tc	853.83	K	Joback Method
tf	395.02	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.45	J/mol×K	669.29	Joback Method
cpg	528.39	J/mol×K	823.08	Joback Method
cpg	519.03	J/mol×K	792.32	Joback Method
cpg	509.07	J/mol×K	761.56	Joback Method
cpg	498.50	J/mol×K	730.80	Joback Method
cpg	487.29	J/mol×K	700.05	Joback Method
cpg	537.14	J/mol×K	853.83	Joback Method
dvisc	0.0000383	Pa×s	669.29	Joback Method
dvisc	0.0000593	Pa×s	623.58	Joback Method
dvisc	0.0000984	Pa×s	577.87	Joback Method

dvisc	0.0001779	Pa×s	532.15	Joback Method
dvisc	0.0003598	Pa×s	486.44	Joback Method
dvisc	0.0008417	Pa×s	440.73	Joback Method
dvisc	0.0023975	Pa×s	395.02	Joback Method

Sources

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=R106699&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume