Dimethyl 3-hydroxy-3-methylpentane-1,5-dioate

Other names: Pentanedioic acid, 3-hydroxy-3-methyl-, dimethyl ester
dimethyl 3-hydroxy-3-methylglutarate

Inchi: InChI=1S/C8H14O5/c1-8(11,4-6(9)12-2)5-7(10)13-3/h11H,4-5H2,1-3H3

InchiKey: ANEMYUYZEOZEJW-UHFFFAOYSA-N

Formula: C8H14O5

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

Mol. weight [g/mol]: 190.19

CAS: 56652-39-2

Physical Properties

Property code	Value	Unit	Source
gf	-585.34	kJ/mol	Joback Method
hf	-859.03	kJ/mol	Joback Method
hfus	18.72	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-0.27		Crippen Method
logp	-0.136		Crippen Method
mcvol	144.330	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	1191.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1191.00		NIST Webbook
tb	623.97	K	Joback Method
tc	808.40	K	Joback Method
tf	387.48	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.01	J/mol×K	623.97	Joback Method
cpg	386.31	J/mol×K	654.71	Joback Method
cpg	396.07	J/mol×K	685.45	Joback Method
cpg	405.32	J/mol×K	716.18	Joback Method

cpg	414.05	J/mol×K	746.92	Joback Method
cpg	422.28	J/mol×K	777.66	Joback Method
cpg	430.00	J/mol×K	808.40	Joback Method
dvisc	0.0024147	Pa×s	387.48	Joback Method
dvisc	0.0009857	Pa×s	426.90	Joback Method
dvisc	0.0004681	Pa×s	466.31	Joback Method
dvisc	0.0002497	Pa×s	505.73	Joback Method
dvisc	0.0001459	Pa×s	545.14	Joback Method
dvisc	0.0000916	Pa×s	584.56	Joback Method
dvisc	0.0000610	Pa×s	623.97	Joback Method

Sources

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=C56652392&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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