Pentanedioic acid, 3-hydroxy-, dimethyl ester

Other names: Glutaric acid, 3-hydroxy-, dimethyl ester
Dimethyl 3-hydroxyglutarate
Inchi: InChI=1S/C7H12O5/c1-11-6(9)3-5(8)4-7(10)12-2/h5,8H,3-4H2,1-2H3
InchiKey: CUPGMRSSZADEIW-UHFFFAOYSA-N
Formula: C7H12O5
SMILES: COC(=O)CC(O)CC(=O)OC
Mol. weight [g/mol]: 176.17
CAS: 7250-55-7

Physical Properties

Property code	Value	Unit	Source
gf	-599.04	kJ/mol	Joback Method
hf	-834.92	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	65.78	kJ/mol	Joback Method
log10ws	0.15		Crippen Method
logp	-0.527		Crippen Method
mcvol	130.240	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
tb	603.88	K	Joback Method
tc	784.28	K	Joback Method
tf	358.79	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.66	J/mol×K	603.88	Joback Method
cpg	335.00	J/mol×K	633.95	Joback Method
cpg	343.95	J/mol×K	664.01	Joback Method
cpg	352.49	J/mol×K	694.08	Joback Method
cpg	360.63	J/mol×K	724.15	Joback Method
cpg	368.34	J/mol×K	754.22	Joback Method
cpg	375.62	J/mol×K	784.28	Joback Method

dvisc	0.0038673	Pa×s	358.79	Joback Method
dvisc	0.0014417	Pa×s	399.64	Joback Method
dvisc	0.0006454	Pa×s	440.49	Joback Method
dvisc	0.0003312	Pa×s	481.34	Joback Method
dvisc	0.0001886	Pa×s	522.18	Joback Method
dvisc	0.0001166	Pa×s	563.03	Joback Method
dvisc	0.0000769	Pa×s	603.88	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=C7250557&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