Methyl 3,3-dimethoxypropionate

Other names: Propanoic acid, 3,3-dimethoxy-, methyl ester
Inchi: InChI=1S/C6H12O4/c1-8-5(7)4-6(9-2)10-3/h6H,4H2,1-3H3
InchiKey: SMCVPMKCDDNUCQ-UHFFFAOYSA-N
Formula: C6H12O4
SMILES: COC(=O)CC(OC)OC
Mol. weight [g/mol]: 148.16
CAS: 7424-91-1

Physical Properties

Property code	Value	Unit	Source
gf	-446.72	kJ/mol	Joback Method
hf	-681.69	kJ/mol	Joback Method
hfus	12.94	kJ/mol	Joback Method
hvap	42.54	kJ/mol	Joback Method
log10ws	0.02		Crippen Method
logp	0.168		Crippen Method
mcvol	114.580	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	457.37	K	Joback Method
tc	638.22	K	Joback Method
tf	259.00	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.97	J/mol×K	457.37	Joback Method
cpg	253.90	J/mol×K	487.51	Joback Method
cpg	263.61	J/mol×K	517.65	Joback Method
cpg	273.08	J/mol×K	547.79	Joback Method
cpg	282.29	J/mol×K	577.94	Joback Method
cpg	291.23	J/mol×K	608.08	Joback Method
cpg	299.88	J/mol×K	638.22	Joback Method
dvisc	0.0025035	Pa×s	259.00	Joback Method

dvisc	0.0012851	Pa×s	292.06	Joback Method
dvisc	0.0007555	Pa×s	325.12	Joback Method
dvisc	0.0004899	Pa×s	358.19	Joback Method
dvisc	0.0003418	Pa×s	391.25	Joback Method
dvisc	0.0002523	Pa×s	424.31	Joback Method
dvisc	0.0001945	Pa×s	457.37	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.20	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7424911&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume