Dimethylpropanedioic acid dimethyl ester

Inchi: InChI=1S/C7H12O4/c1-7(2,5(8)10-3)6(9)11-4/h1-4H3
InchiKey: CAFVGIPKHPBMJS-UHFFFAOYSA-N
Formula: C7H12O4
SMILES: COC(=O)C(C)(C)C(=O)OC
Mol. weight [g/mol]: 160.17
CAS: 6065-54-9

Physical Properties

Property code	Value	Unit	Source
chl	-3611.10 ± 0.42	kJ/mol	NIST Webbook
gf	-456.94	kJ/mol	Joback Method
hf	-802.74 ± 0.79	kJ/mol	NIST Webbook
hfl	-858.43 ± 0.42	kJ/mol	NIST Webbook
hfus	12.05	kJ/mol	Joback Method
hvap	55.69 ± 0.79	kJ/mol	NIST Webbook
hvap	55.70	kJ/mol	NIST Webbook
log10ws	-0.24		Crippen Method
logp	0.359		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	508.91	K	Joback Method
tc	706.01	K	Joback Method
tf	315.39	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.74	J/mol×K	508.91	Joback Method
cpg	341.51	J/mol×K	706.01	Joback Method
cpg	332.83	J/mol×K	673.16	Joback Method
cpg	323.65	J/mol×K	640.31	Joback Method
cpg	313.95	J/mol×K	607.46	Joback Method
cpg	303.74	J/mol×K	574.61	Joback Method

cpg	293.00	J/mol×K	541.76	Joback Method
cpl	259.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0014058	Pa×s	347.64	Joback Method
dvisc	0.0002384	Pa×s	508.91	Joback Method
dvisc	0.0003088	Pa×s	476.66	Joback Method
dvisc	0.0004154	Pa×s	444.40	Joback Method
dvisc	0.0005852	Pa×s	412.15	Joback Method
dvisc	0.0008739	Pa×s	379.90	Joback Method
dvisc	0.0024923	Pa×s	315.39	Joback Method
hvapt	55.60 ± 0.80	kJ/mol	292.50	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6065549&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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