2-Hydroxy-3-methoxycarbonyl-pentanedioic acid dimethyl ester

Inchi: InChI=1S/C8H14O6/c1-12-5(4-6(9)13-2)7(10)8(11)14-3/h5,7,10H,4H2,1-3H3
InchiKey: BJOASXQKJRDION-UHFFFAOYSA-N
Formula: C8H14O6
SMILES: COC(=O)CC(OC)C(O)C(=O)OC
Mol. weight [g/mol]: 206.19

Physical Properties

Property code	Value	Unit	Source
gf	-698.06	kJ/mol	Joback Method
hf	-993.06	kJ/mol	Joback Method
hfus	20.28	kJ/mol	Joback Method
hvap	70.03	kJ/mol	Joback Method
log10ws	0.53		Crippen Method
logp	-0.902		Crippen Method
mcvol	150.200	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	1435.00		NIST Webbook
tb	648.74	K	Joback Method
tc	830.16	K	Joback Method
tf	377.29	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.46	J/mol×K	648.74	Joback Method
cpg	407.81	J/mol×K	678.98	Joback Method
cpg	417.68	J/mol×K	709.21	Joback Method
cpg	427.06	J/mol×K	739.45	Joback Method
cpg	435.93	J/mol×K	769.69	Joback Method
cpg	444.28	J/mol×K	799.92	Joback Method
cpg	452.10	J/mol×K	830.16	Joback Method
dvisc	0.0026939	Pa×s	377.29	Joback Method
dvisc	0.0009380	Pa×s	422.53	Joback Method

dvisc	0.0004005	Pa×s	467.77	Joback Method
dvisc	0.0001987	Pa×s	513.01	Joback Method
dvisc	0.0001105	Pa×s	558.26	Joback Method
dvisc	0.0000670	Pa×s	603.50	Joback Method
dvisc	0.0000436	Pa×s	648.74	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=R247735&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume