2-Hydroxypropane-1,2,3-tricarboxylic acid, dimethyl ester

Other names: (R)-3-Hydroxy-5-methoxy-3-(methoxycarbonyl)-5-oxopentanoic acid
Inchi: InChI=1S/C8H12O7/c1-14-6(11)4-8(13,3-5(9)10)7(12)15-2/h13H,3-4H2,1-2H3,(H,9,10)
InchiKey: OMIHCBSQSYMFDP-UHFFFAOYSA-N
Formula: C8H12O7
SMILES: COC(=O)CC(O)(CC(=O)O)C(=O)OC
Mol. weight [g/mol]: 220.18

Physical Properties

Property code	Value	Unit	Source
gf	-851.08	kJ/mol	Joback Method
hf	-1123.84	kJ/mol	Joback Method
hfus	24.41	kJ/mol	Joback Method
hvap	90.52	kJ/mol	Joback Method
log10ws	0.63		Crippen Method
logp	-1.072		Crippen Method
mcvol	151.770	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	1563.00		NIST Webbook
tb	770.02	K	Joback Method
tc	957.96	K	Joback Method
tf	498.23	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.94	J/mol×K	770.02	Joback Method
cpg	438.59	J/mol×K	801.34	Joback Method
cpg	445.70	J/mol×K	832.67	Joback Method
cpg	452.28	J/mol×K	863.99	Joback Method
cpg	458.35	J/mol×K	895.31	Joback Method
cpg	463.90	J/mol×K	926.64	Joback Method
cpg	468.94	J/mol×K	957.96	Joback Method
dvisc	0.0004182	Pa×s	498.23	Joback Method

dvisc	0.0001605	Pa×s	543.53	Joback Method
dvisc	0.0000714	Pa×s	588.83	Joback Method
dvisc	0.0000356	Pa×s	634.12	Joback Method
dvisc	0.0000195	Pa×s	679.42	Joback Method
dvisc	0.0000115	Pa×s	724.72	Joback Method
dvisc	0.0000072	Pa×s	770.02	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=U378712&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