Pentanedioic acid, 3-hydroxy-3-(methoxycarbonylmethyl), dimethyl ester

InChI: InChI=1S/C10H16O7/c1-15-7(11)4-10(14,5-8(12)16-2)6-9(13)17-3/h14H,4-6H2,1-3H3
InChIKey: INSYEQUXCNXBRN-UHFFFAOYSA-N
Formula: C10H16O7
SMILES: COC(=O)CC(O)(CC(=O)OC)CC(=O)OC
Mol. weight [g/mol]: 248.23

Physical Properties

Property code	Value	Unit	Source
gf	-802.42	kJ/mol	Joback Method
hf	-1145.11	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	80.70	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	-0.593		Crippen Method
mcvol	179.950	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	746.02	K	Joback Method
tc	935.24	K	Joback Method
tf	482.18	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.56	J/mol×K	746.02	Joback Method
cpg	523.93	J/mol×K	777.56	Joback Method
cpg	533.62	J/mol×K	809.09	Joback Method
cpg	542.64	J/mol×K	840.63	Joback Method
cpg	550.99	J/mol×K	872.17	Joback Method
cpg	558.67	J/mol×K	903.70	Joback Method
cpg	565.67	J/mol×K	935.24	Joback Method
dvisc	0.0005835	Pa×s	482.18	Joback Method

dvisc	0.0002761	Pa×s	526.15	Joback Method
dvisc	0.0001466	Pa×s	570.13	Joback Method
dvisc	0.0000853	Pa×s	614.10	Joback Method
dvisc	0.0000533	Pa×s	658.07	Joback Method
dvisc	0.0000353	Pa×s	702.05	Joback Method
dvisc	0.0000246	Pa×s	746.02	Joback Method

Sources

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=R106708&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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