Pentanedioic acid, 3-ethyl-3-hydroxy, dimethyl ester

Inchi: InChI=1S/C9H16O5/c1-4-9(12,5-7(10)13-2)6-8(11)14-3/h12H,4-6H2,1-3H3
InchiKey: OPEYCEQEAPLEOV-UHFFFAOYSA-N
Formula: C9H16O5
SMILES: CCC(O)(CC(=O)OC)CC(=O)OC
Mol. weight [g/mol]: 204.22

Physical Properties

Property code	Value	Unit	Source
gf	-576.92	kJ/mol	Joback Method
hf	-879.67	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.254		Crippen Method
mcvol	158.420	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1248.00		NIST Webbook
tb	646.85	K	Joback Method
tc	829.81	K	Joback Method
tf	398.75	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.72	J/mol×K	646.85	Joback Method
cpg	474.11	J/mol×K	799.31	Joback Method
cpg	465.35	J/mol×K	768.82	Joback Method
cpg	456.03	J/mol×K	738.33	Joback Method
cpg	446.16	J/mol×K	707.84	Joback Method
cpg	435.73	J/mol×K	677.34	Joback Method
cpg	482.35	J/mol×K	829.81	Joback Method
dvisc	0.0000502	Pa×s	646.85	Joback Method
dvisc	0.0000754	Pa×s	605.50	Joback Method

dvisc	0.0001202	Pa×s	564.15	Joback Method
dvisc	0.0002064	Pa×s	522.80	Joback Method
dvisc	0.0003887	Pa×s	481.45	Joback Method
dvisc	0.0008248	Pa×s	440.10	Joback Method
dvisc	0.0020454	Pa×s	398.75	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=R106684&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