2-Hydroxyglutaric acid diethyl ester

Other names: Diethyl 2-hydroxyglutarate
Inchi: InChI=1S/C9H16O5/c1-3-13-8(11)6-5-7(10)9(12)14-4-2/h7,10H,3-6H2,1-2H3
InchiKey: DYLHSDCNOUDICA-UHFFFAOYSA-N
Formula: C9H16O5
SMILES: CCOC(=O)CCC(O)C(=O)OCC
Mol. weight [g/mol]: 204.22
CAS: 69134-53-8

Physical Properties

Property code	Value	Unit	Source
gf	-582.20	kJ/mol	Joback Method
hf	-876.20	kJ/mol	Joback Method
hfus	25.21	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.254		Crippen Method
mcvol	158.420	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
ripol	2195.00		NIST Webbook
tb	649.64	K	Joback Method
tc	827.66	K	Joback Method
tf	381.33	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.95	J/mol×K	649.64	Joback Method
cpg	432.85	J/mol×K	679.31	Joback Method
cpg	443.26	J/mol×K	708.98	Joback Method
cpg	453.15	J/mol×K	738.65	Joback Method
cpg	462.54	J/mol×K	768.32	Joback Method
cpg	471.41	J/mol×K	797.99	Joback Method
cpg	479.77	J/mol×K	827.66	Joback Method

dvisc	0.0027887	Pa×s	381.33	Joback Method
dvisc	0.0010206	Pa×s	426.05	Joback Method
dvisc	0.0004521	Pa×s	470.77	Joback Method
dvisc	0.0002307	Pa×s	515.49	Joback Method
dvisc	0.0001310	Pa×s	560.20	Joback Method
dvisc	0.0000809	Pa×s	604.92	Joback Method
dvisc	0.0000534	Pa×s	649.64	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=C69134538&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume