Diethyl bis(hydroxymethyl)malonate

Other names: Propanedioic acid, bis(hydroxymethyl)-, diethyl ester
Inchi: InChI=1S/C9H16O6/c1-3-14-7(12)9(5-10,6-11)8(13)15-4-2/h10-11H,3-6H2,1-2H3
InchiKey: WIOHBOKEUIHYIC-UHFFFAOYSA-N
Formula: C9H16O6
SMILES: CCOC(=O)C(CO)(CO)C(=O)OCC
Mol. weight [g/mol]: 220.22
CAS: 20605-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-713.74	kJ/mol	Joback Method
hf	-1031.90	kJ/mol	Joback Method
hfus	25.40	kJ/mol	Joback Method
hvap	86.00	kJ/mol	Joback Method
log10ws	0.40		Crippen Method
logp	-0.916		Crippen Method
mcvol	164.290	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	739.03	K	Joback Method
tc	919.46	K	Joback Method
tf	459.57	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.01	J/mol×K	739.03	Joback Method
cpg	515.28	J/mol×K	889.39	Joback Method
cpg	508.07	J/mol×K	859.32	Joback Method
cpg	500.35	J/mol×K	829.25	Joback Method
cpg	492.11	J/mol×K	799.17	Joback Method
cpg	483.33	J/mol×K	769.10	Joback Method
cpg	521.97	J/mol×K	919.46	Joback Method
dvisc	0.0000077	Pa×s	739.03	Joback Method

dvisc	0.0000127	Pa×s	692.45	Joback Method
dvisc	0.0000228	Pa×s	645.88	Joback Method
dvisc	0.0000445	Pa×s	599.30	Joback Method
dvisc	0.0000975	Pa×s	552.72	Joback Method
dvisc	0.0002467	Pa×s	506.15	Joback Method
dvisc	0.0007531	Pa×s	459.57	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=C20605010&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume