Pentanedioic acid, 3-oxo-, diethyl ester

Other names:	Glutaric acid, 3-oxo-, diethyl ester
	Acetonedicarboxylic acid, diethyl ester
	Butanoic acid, (ethoxycarbonyl)-3-oxo-, ethyl ester
	Diethyl «beta»-oxoglutarate
	Diethyl acetonedicarboxylate
	Diethyl 1,3-acetonedicarboxylate
	Diethyl 3-oxoglutarate
	Diethyl 3-oxopentanedioate
	Ethyl 3-oxoglutarate
	3-Oxoglutaric acid, diethyl ester
	3-Oxopentanedioic acid, diethyl ester
	Ethyl acetonedicarboxylate
	Diethyl «beta»-ketoglutarate
	NSC 9013
	Pentanedioic acid, 3-oxo-, 1,5-diethyl ester
Inchi:	InChI=1S/C9H14O5/c1-3-13-8(11)5-7(10)6-9(12)14-4-2/h3-6H2,1-2H3
InchiKey:	ZSANYRMTSBBUCA-UHFFFAOYSA-N
Formula:	C9H14O5
SMILES:	CCOC(=O)CC(=O)CC(=O)OCC
Mol. weight [g/mol]:	202.20
CAS:	105-50-0

Physical Properties

Property code	Value	Unit	Source
gf	-571.86	kJ/mol	Joback Method
hf	-831.27	kJ/mol	Joback Method
hfus	26.24	kJ/mol	Joback Method
hvap	60.69	kJ/mol	Joback Method
log10ws	-0.60		Crippen Method
logp	0.462		Crippen Method
mcvol	154.120	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
tb	523.20	K	NIST Webbook
tc	801.38	K	Joback Method
tf	385.44	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.88	J/mol×K	611.77	Joback Method
cpg	437.10	J/mol×K	769.78	Joback Method
cpg	427.75	J/mol×K	738.17	Joback Method
cpg	417.85	J/mol×K	706.57	Joback Method
cpg	407.40	J/mol×K	674.97	Joback Method
cpg	396.41	J/mol×K	643.37	Joback Method
cpg	445.88	J/mol×K	801.38	Joback Method
dvisc	0.0002140	Pa×s	611.77	Joback Method
dvisc	0.0002693	Pa×s	574.05	Joback Method
dvisc	0.0003501	Pa×s	536.33	Joback Method
dvisc	0.0004734	Pa×s	498.61	Joback Method
dvisc	0.0006728	Pa×s	460.88	Joback Method
dvisc	0.0010179	Pa×s	423.16	Joback Method
dvisc	0.0016699	Pa×s	385.44	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C105500&Units=SI

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