Propanedioic acid, oxo-, diethyl ester

Other names:	Mesoxalic acid, diethyl ester
	Diethyl mesoxalate
	Diethyl oxomalonate
	Ethyl mesoxalate
	Diethyl ketomalonate
	Ketomalonic acid diethyl ester
Inchi:	InChI=1S/C7H10O5/c1-3-11-6(9)5(8)7(10)12-4-2/h3-4H2,1-2H3
InchiKey:	DBKKFIIYQGGHJO-UHFFFAOYSA-N
Formula:	C7H10O5
SMILES:	CCOC(=O)C(=O)C(=O)OCC
Mol. weight [g/mol]:	174.15
CAS:	609-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-588.70	kJ/mol	Joback Method
hf	-789.99	kJ/mol	Joback Method
hfus	21.06	kJ/mol	Joback Method
hvap	56.23	kJ/mol	Joback Method
log10ws	0.24		Crippen Method
logp	-0.318		Crippen Method
mcvol	125.940	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
tb	482.20	K	NIST Webbook
tc	760.26	K	Joback Method
tf	362.90	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.09	J/mol×K	566.01	Joback Method
cpg	301.83	J/mol×K	598.38	Joback Method
cpg	311.16	J/mol×K	630.76	Joback Method

cpg	320.07	J/mol×K	663.13	Joback Method
cpg	328.54	J/mol×K	695.51	Joback Method
cpg	336.57	J/mol×K	727.88	Joback Method
cpg	344.14	J/mol×K	760.26	Joback Method
dvisc	0.0017994	Pa×s	362.90	Joback Method
dvisc	0.0011370	Pa×s	396.75	Joback Method
dvisc	0.0007723	Pa×s	430.60	Joback Method
dvisc	0.0005550	Pa×s	464.46	Joback Method
dvisc	0.0004171	Pa×s	498.31	Joback Method
dvisc	0.0003251	Pa×s	532.16	Joback Method
dvisc	0.0002610	Pa×s	566.01	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=C609096&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

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