Diethyl diethylmalonate

Other names:	Diethylmalonic acid diethyl ester
	Propanedioic acid, diethyl-, diethyl ester
	Diethylmalonate diethyl ester
	Diethylmalonic ester
	Malonic acid, diethyl-, diethyl ester
Inchi:	InChI=1S/C11H20O4/c1-5-11(6-2,9(12)14-7-3)10(13)15-8-4/h5-8H2,1-4H3
InchiKey:	ZKBBUZRGPULIRN-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CCOC(=O)C(CC)(CC)C(=O)OCC
Mol. weight [g/mol]:	216.27
CAS:	77-25-8

Physical Properties

Property code	Value	Unit	Source
gf	-423.26	kJ/mol	Joback Method
hf	-768.72	kJ/mol	Joback Method
hfus	22.41	kJ/mol	Joback Method
hvap	57.10	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.919		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
tb	503.20	K	NIST Webbook
tc	788.01	K	Joback Method
tf	360.47	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.93	J/mol×K	788.01	Joback Method
cpg	533.85	J/mol×K	756.75	Joback Method
cpg	522.10	J/mol×K	725.48	Joback Method
cpg	509.68	J/mol×K	694.22	Joback Method

cpg	496.56	J/mol×K	662.96	Joback Method
cpg	482.73	J/mol×K	631.69	Joback Method
cpg	468.19	J/mol×K	600.43	Joback Method
dvisc	0.0019947	Pa×s	360.47	Joback Method
dvisc	0.0001518	Pa×s	600.43	Joback Method
dvisc	0.0002001	Pa×s	560.44	Joback Method
dvisc	0.0002751	Pa×s	520.44	Joback Method
dvisc	0.0003989	Pa×s	480.45	Joback Method
dvisc	0.0006188	Pa×s	440.46	Joback Method
dvisc	0.0010480	Pa×s	400.46	Joback Method
hvapt	68.50	kJ/mol	438.50	NIST Webbook

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=C77258&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
hvapt: Enthalpy of vaporization at a given temperature
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