Propanedioic acid, ethyl-, diethyl ester

Other names:	Malonic acid, ethyl-, diethyl ester
	Diethyl ethylmalonate
	Diethyl 2-ethylmalonate
	Ethyl diethylmalonate
	Ethylmalonic acid diethyl ester
Inchi:	InChI=1S/C9H16O4/c1-4-7(8(10)12-5-2)9(11)13-6-3/h7H,4-6H2,1-3H3
InchiKey:	VQAZCUCWHIIFGE-UHFFFAOYSA-N
Formula:	C9H16O4
SMILES:	CCOC(=O)C(CC)C(=O)OCC
Mol. weight [g/mol]:	188.22
CAS:	133-13-1

Physical Properties

Property code	Value	Unit	Source
gf	-445.38	kJ/mol	Joback Method
hf	-723.97	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.139		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1148.00		NIST Webbook
tb	557.46	K	Joback Method
tc	742.78	K	Joback Method
tf	320.51	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.72	J/mol×K	742.78	Joback Method
cpg	368.40	J/mol×K	557.46	Joback Method
cpg	381.08	J/mol×K	588.35	Joback Method

cpg	393.25	J/mol×K	619.23	Joback Method
cpg	404.90	J/mol×K	650.12	Joback Method
cpg	416.03	J/mol×K	681.01	Joback Method
cpg	426.64	J/mol×K	711.90	Joback Method
dvisc	0.0001960	Pa×s	557.46	Joback Method
dvisc	0.0025423	Pa×s	320.51	Joback Method
dvisc	0.0013123	Pa×s	360.00	Joback Method
dvisc	0.0007719	Pa×s	399.49	Joback Method
dvisc	0.0004996	Pa×s	438.99	Joback Method
dvisc	0.0003474	Pa×s	478.48	Joback Method
dvisc	0.0002553	Pa×s	517.97	Joback Method
hvapt	55.30	kJ/mol	404.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.20	K	0.70	NIST Webbook

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=C133131&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume