Diethyl diallylmalonate

Other names:	Diallylmalonic acid diethyl ester
	Propanedioic acid, di-2-propenyl-, diethyl ester
	Malonic acid, diallyl-, diethyl ester
Inchi:	InChI=1S/C13H20O4/c1-5-9-13(10-6-2,11(14)16-7-3)12(15)17-8-4/h5-6H,1-2,7-10H2,3-4
InchiKey:	LYUUVYQGUMRKOV-UHFFFAOYSA-N
Formula:	C13H20O4
SMILES:	C=CCC(CC=C)(C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]:	240.30
CAS:	3195-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-230.74	kJ/mol	Joback Method
hf	-559.14	kJ/mol	Joback Method
hfus	25.03	kJ/mol	Joback Method
hvap	60.21	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.251		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
tb	639.55	K	Joback Method
tc	829.50	K	Joback Method
tf	379.49	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.47	J/mol×K	639.55	Joback Method
cpg	541.01	J/mol×K	671.21	Joback Method
cpg	554.75	J/mol×K	702.87	Joback Method
cpg	567.73	J/mol×K	734.52	Joback Method
cpg	579.96	J/mol×K	766.18	Joback Method
cpg	591.47	J/mol×K	797.84	Joback Method

cpg	602.28	J/mol×K	829.50	Joback Method
dvisc	0.0016514	Pa×s	379.49	Joback Method
dvisc	0.0008680	Pa×s	422.83	Joback Method
dvisc	0.0005142	Pa×s	466.18	Joback Method
dvisc	0.0003330	Pa×s	509.52	Joback Method
dvisc	0.0002308	Pa×s	552.86	Joback Method
dvisc	0.0001688	Pa×s	596.21	Joback Method
dvisc	0.0001287	Pa×s	639.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.20	K	1.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3195242&Units=SI
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

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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume