Diethyl allylmalonate

Other names:	Diethyl allylmalonate
	Diethyl prop-2-enylpropanedioate
	Diethyl 2-(prop-2-enyl)malonate
	Diethyl 2-allylmalonate
	Ethyl allylmalonate
	Malonic acid, allyl-, diethyl ester
	Diethyl 2-(2-propenyl)-1,3-propanedioate
	2-Allylmalonic acid diethyl ester
	NSC 67393
	NSC 8777
	Propanedioic acid, 2-(2-propen-1-yl)-, 1,3-diethyl ester
Inchi:	InChI=1S/C10H16O4/c1-4-7-8(9(11)13-5-2)10(12)14-6-3/h4,8H,1,5-7H2,2-3H3
InchiKey:	GDWAYKGILJJNBB-UHFFFAOYSA-N
Formula:	C10H16O4
SMILES:	C=CCC(C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]:	200.23

Physical Properties

Property code	Value	Unit	Source
af	0.5229		Cheméo Relay (1.0)
hf	-774.63	kJ/mol	Cheméo Relay (1.0)
hfus	22.43	kJ/mol	Joback Method
hvap	66.72	kJ/mol	Cheméo Relay (1.0)
ie	9.49	eV	Cheméo Relay (1.0)
log10ws	-1.74		Cheméo Relay (1.0)
logp	1.305		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	498.64	K	Cheméo Relay (1.0)
tc	672.43	K	Cheméo Relay (1.0)
tf	214.75	K	Cheméo Relay (1.0)
vc	0.575	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.75	J/mol×K	577.02	Joback Method
cpg	464.55	J/mol×K	763.66	Joback Method
cpg	454.50	J/mol×K	732.55	Joback Method
cpg	443.89	J/mol×K	701.45	Joback Method
cpg	432.70	J/mol×K	670.34	Joback Method
cpg	420.95	J/mol×K	639.23	Joback Method
cpg	408.63	J/mol×K	608.13	Joback Method
dvisc	0.0004624	Pa×s	453.52	Joback Method
dvisc	0.0001833	Pa×s	577.02	Joback Method
dvisc	0.0002380	Pa×s	535.85	Joback Method
dvisc	0.0003227	Pa×s	494.69	Joback Method
dvisc	0.0023329	Pa×s	330.02	Joback Method
dvisc	0.0007121	Pa×s	412.35	Joback Method
dvisc	0.0012068	Pa×s	371.19	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2049801&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
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