

Propanedioic acid, 2-propenyl-, diethyl ester

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
CAS:	2049-80-1

Physical Properties

Property code	Value	Unit	Source
gf	-349.12	kJ/mol	Joback Method
hf	-619.18	kJ/mol	Joback Method
hfus	22.43	kJ/mol	Joback Method
hvap	55.11	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.305		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	495.70	K	NIST Webbook
tc	763.66	K	Joback Method
tf	330.02	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.20	K	0.80	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=C2049801&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
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

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