PROPANEDIOIC ACID, DI-2-PROPENYL-, DIETHYL ESTER

Other names: Diallylmalonic acid diethyl ester
Malonic acid, diallyl-, diethyl ester
Propanedioic acid, di-2-propenyl-, 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

Physical Properties

Property code	Value	Unit	Source
af	0.5508		Cheméo Relay (1.0)
hf	-711.01	kJ/mol	Cheméo Relay (1.0)
hfus	25.03	kJ/mol	Joback Method
hvap	64.35	kJ/mol	Cheméo Relay (1.0)
ie	9.19	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	2.251		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
tb	528.13	K	Cheméo Relay (1.0)
tc	705.12	K	Cheméo Relay (1.0)
tf	266.48	K	Cheméo Relay (1.0)
vc	0.674	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.47	J/mol×K	639.55	Joback Method
cpg	602.28	J/mol×K	829.50	Joback Method
cpg	591.47	J/mol×K	797.84	Joback Method
cpg	579.96	J/mol×K	766.18	Joback Method
cpg	567.73	J/mol×K	734.52	Joback Method
cpg	554.75	J/mol×K	702.87	Joback Method

cpg	541.01	J/mol×K	671.21	Joback Method
dvisc	0.0003330	Pa×s	509.52	Joback Method
dvisc	0.0001287	Pa×s	639.55	Joback Method
dvisc	0.0001688	Pa×s	596.21	Joback Method
dvisc	0.0002308	Pa×s	552.86	Joback Method
dvisc	0.0016514	Pa×s	379.49	Joback Method
dvisc	0.0005142	Pa×s	466.18	Joback Method
dvisc	0.0008680	Pa×s	422.83	Joback Method

Pressure Dependent Properties

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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3195242&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

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