DIVINYL ADIPATE

Other names:	Hexanedioic acid, diethenyl ester
	Divinyladipate
	Hexanedionic acid, diethenyl ester
Inchi:	InChI=1S/C10H14O4/c1-3-13-9(11)7-5-6-8-10(12)14-4-2/h3-4H,1-2,5-8H2
InchiKey:	JZQAAQZDDMEFGZ-UHFFFAOYSA-N
Formula:	C10H14O4
SMILES:	C=COC(=O)CCCCC(=O)OC=C
Mol. weight [g/mol]:	198.22

Physical Properties

Property code	Value	Unit	Source
af	0.7403		Cheméo Relay (1.0)
hf	-646.96	kJ/mol	Cheméo Relay (1.0)
hfus	24.67	kJ/mol	Joback Method
hvap	69.60	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-1.96		Cheméo Relay (1.0)
logp	1.920		Crippen Method
mcvol	158.040	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1295.00		NIST Webbook
rinpol	1295.00		NIST Webbook
tb	507.24	K	Cheméo Relay (1.0)
tc	670.49	K	Cheméo Relay (1.0)
tf	261.47	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	375.22	J/mol×K	574.14	Joback Method
cpg	439.03	J/mol×K	760.60	Joback Method
cpg	429.73	J/mol×K	729.52	Joback Method
cpg	419.89	J/mol×K	698.44	Joback Method

cpg	409.53	J/mol×K	667.37	Joback Method
cpg	398.63	J/mol×K	636.29	Joback Method
cpg	387.19	J/mol×K	605.22	Joback Method
dvisc	0.0004567	Pa×s	458.70	Joback Method
dvisc	0.0002023	Pa×s	574.14	Joback Method
dvisc	0.0002552	Pa×s	535.66	Joback Method
dvisc	0.0003338	Pa×s	497.18	Joback Method
dvisc	0.0017838	Pa×s	343.26	Joback Method
dvisc	0.0006618	Pa×s	420.22	Joback Method
dvisc	0.0010336	Pa×s	381.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.00	K	0.80	NIST Webbook

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4074902&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
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