Diallyl suberate

Inchi: InChI=1S/C14H22O4/c1-3-11-17-13(15)9-7-5-6-8-10-14(16)18-12-4-2/h3-4H,1-2,5-12H2
InchiKey: QFUAOHZJDCNMNB-UHFFFAOYSA-N
Formula: C14H22O4
SMILES: C=CCOC(=O)CCCCCCC(=O)OCC=C
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-225.16	kJ/mol	Joback Method
hf	-571.03	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	63.73	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.785		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	665.66	K	Joback Method
tc	846.06	K	Joback Method
tf	388.34	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.88	J/mol×K	665.66	Joback Method
cpg	641.73	J/mol×K	816.00	Joback Method
cpg	629.94	J/mol×K	785.93	Joback Method
cpg	617.47	J/mol×K	755.86	Joback Method
cpg	604.31	J/mol×K	725.79	Joback Method
cpg	590.45	J/mol×K	695.73	Joback Method
cpg	652.84	J/mol×K	846.06	Joback Method
dvisc	0.0001321	Pa×s	665.66	Joback Method

dvisc	0.0001697	Pa×s	619.44	Joback Method
dvisc	0.0002270	Pa×s	573.22	Joback Method
dvisc	0.0003196	Pa×s	527.00	Joback Method
dvisc	0.0004804	Pa×s	480.78	Joback Method
dvisc	0.0007877	Pa×s	434.56	Joback Method
dvisc	0.0014527	Pa×s	388.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542337&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume