ALLYL OCTYL ETHER

Other names: Allyl octyl ether
Inchi: InChI=1S/C11H22O/c1-3-5-6-7-8-9-11-12-10-4-2/h4H,2-3,5-11H2,1H3
InchiKey: IELYMBBIHQDONA-UHFFFAOYSA-N
Formula: C11H22O
SMILES: C=CCOCCCCCCCC
Mol. weight [g/mol]: 170.30

Physical Properties

Property code	Value	Unit	Source
af	0.5582		Cheméo Relay (1.0)
gf	24.58	kJ/mol	Joback Method
hf	-283.55	kJ/mol	Cheméo Relay (1.0)
hfus	24.15	kJ/mol	Joback Method
hvap	55.04	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-3.94		Cheméo Relay (1.0)
logp	3.550		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
tb	479.20 ± 1.00	K	NIST Webbook
tc	654.89	K	Cheméo Relay (1.0)
tf	212.20 ± 1.00	K	NIST Webbook
vc	0.625	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.42	J/mol×K	470.18	Joback Method
cpg	385.59	J/mol×K	497.64	Joback Method
cpg	400.22	J/mol×K	525.10	Joback Method
cpg	414.30	J/mol×K	552.56	Joback Method
cpg	427.86	J/mol×K	580.01	Joback Method
cpg	440.91	J/mol×K	607.47	Joback Method
cpg	453.44	J/mol×K	634.93	Joback Method

dvisc	0.0038824	Pa×s	234.20	Joback Method
dvisc	0.0016405	Pa×s	273.53	Joback Method
dvisc	0.0008608	Pa×s	312.86	Joback Method
dvisc	0.0005217	Pa×s	352.19	Joback Method
dvisc	0.0003496	Pa×s	391.52	Joback Method
dvisc	0.0002521	Pa×s	430.85	Joback Method
dvisc	0.0001920	Pa×s	470.18	Joback Method

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=C3295974&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
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
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