

Allyl ethyl ether

Other names:	1-Propene, 3-ethoxy- 3-ETHOXY-1-PROPENE 3-Ethoxypropene <chem>CH3CH2OCH2CH=CH2</chem> Ether, allyl ethyl Ethyl 2-propenyl ether Ethyl allyl ether UN 2335
Inchi:	InChI=1S/C5H10O/c1-3-5-6-4-2/h3H,1,4-5H2,2H3
InchiKey:	OJPSFJLSZZTSDF-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	<chem>C=CCOCC</chem>
Mol. weight [g/mol]:	86.13
CAS:	557-31-3

Physical Properties

Property code	Value	Unit	Source
affp	833.70	kJ/mol	NIST Webbook
basg	804.50	kJ/mol	NIST Webbook
gf	-25.94	kJ/mol	Joback Method
hf	-153.32	kJ/mol	Joback Method
hfus	8.61	kJ/mol	Joback Method
hvap	28.46	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	1.209		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	586.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	571.00		NIST Webbook
rinpol	570.00		NIST Webbook
tb	340.00	K	NIST Webbook
tb	335.15 ± 2.00	K	NIST Webbook
tb	340.80	K	KDB
tb	339.20	K	NIST Webbook
tc	518.00 ± 10.00	K	NIST Webbook

tc	518.00	K	KDB
tf	166.58	K	Joback Method
vc	0.315	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.14	J/mol×K	500.59	Joback Method
cpg	135.21	J/mol×K	332.90	Joback Method
cpg	143.28	J/mol×K	360.85	Joback Method
cpg	151.11	J/mol×K	388.80	Joback Method
cpg	158.71	J/mol×K	416.74	Joback Method
cpg	166.08	J/mol×K	444.69	Joback Method
cpg	173.22	J/mol×K	472.64	Joback Method
dvisc	0.0002010	Pa×s	332.90	Joback Method
dvisc	0.0024826	Pa×s	166.58	Joback Method
dvisc	0.0012110	Pa×s	194.30	Joback Method
dvisc	0.0007067	Pa×s	222.02	Joback Method
dvisc	0.0004648	Pa×s	249.74	Joback Method
dvisc	0.0003324	Pa×s	277.46	Joback Method
dvisc	0.0002526	Pa×s	305.18	Joback Method
hvapt	34.60	kJ/mol	322.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1004.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C557313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity

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
hvapt:	Enthalpy of vaporization at a given temperature
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

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