

Ether, ethyl 1-heptenyl, (E)-

Inchi:	InChI=1S/C9H18O/c1-3-5-6-7-8-9-10-4-2/h8-9H,3-7H2,1-2H3/b9-8+
InchiKey:	SDTIAHWPSZKYHU-CMDGGGOBGSA-N
Formula:	C9H18O
SMILES:	CCCCC=COCC
Mol. weight [g/mol]:	142.24
CAS:	16627-11-5

Physical Properties

Property code	Value	Unit	Source
gf	0.12	kJ/mol	Joback Method
hf	-244.09	kJ/mol	Joback Method
hfus	20.46	kJ/mol	Joback Method
hvap	38.00	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	3.117		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
tb	431.90	K	Joback Method
tc	603.05	K	Joback Method
tf	208.34	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.61	J/mol×K	431.90	Joback Method
cpg	346.64	J/mol×K	574.53	Joback Method
cpg	335.02	J/mol×K	546.00	Joback Method
cpg	322.91	J/mol×K	517.48	Joback Method
cpg	310.32	J/mol×K	488.95	Joback Method
cpg	297.22	J/mol×K	460.43	Joback Method
cpg	357.80	J/mol×K	603.05	Joback Method
dvisc	0.0001771	Pa×s	431.90	Joback Method
dvisc	0.0002330	Pa×s	394.64	Joback Method

dvisc	0.0003248	Pa×s	357.38	Joback Method
dvisc	0.0004889	Pa×s	320.12	Joback Method
dvisc	0.0008199	Pa×s	282.86	Joback Method
dvisc	0.0016083	Pa×s	245.60	Joback Method
dvisc	0.0040144	Pa×s	208.34	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16627115&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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