

Ether, isobutyl propenyl, (E)-

Inchi:	InChI=1S/C7H14O/c1-4-5-8-6-7(2)3/h4-5,7H,6H2,1-3H3/b5-4+
InchiKey:	JCCRGQZQICHINY-SNAWJCMRSA-N
Formula:	C7H14O
SMILES:	CC=COCC(C)C
Mol. weight [g/mol]:	114.19
CAS:	13049-22-4

Physical Properties

Property code	Value	Unit	Source
gf	-19.16	kJ/mol	Joback Method
hf	-208.09	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	33.16	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.193		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
tb	385.70	K	Joback Method
tc	562.62	K	Joback Method
tf	170.80	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.90	J/mol×K	385.70	Joback Method
cpg	215.57	J/mol×K	415.19	Joback Method
cpg	226.80	J/mol×K	444.67	Joback Method
cpg	237.60	J/mol×K	474.16	Joback Method
cpg	247.98	J/mol×K	503.65	Joback Method
cpg	257.95	J/mol×K	533.13	Joback Method
cpg	267.51	J/mol×K	562.62	Joback Method
dvisc	0.0065425	Pa×s	170.80	Joback Method
dvisc	0.0021300	Pa×s	206.62	Joback Method

dvisc	0.0009661	Pa×s	242.43	Joback Method
dvisc	0.0005371	Pa×s	278.25	Joback Method
dvisc	0.0003414	Pa×s	314.07	Joback Method
dvisc	0.0002381	Pa×s	349.88	Joback Method
dvisc	0.0001775	Pa×s	385.70	Joback Method

Sources

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=C13049224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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