

(E,E)(1-Butenyl)(1-propenyl)ether

Inchi:	InChI=1S/C7H12O/c1-3-5-7-8-6-4-2/h4-7H,3H2,1-2H3/b6-4+,7-5+
InchiKey:	BDJSOOUWCKJJQE-YDFGWWAZSA-N
Formula:	C7H12O
SMILES:	CC=COC=CCC
Mol. weight [g/mol]:	112.17
CAS:	61463-28-3

Physical Properties

Property code	Value	Unit	Source
gf	63.50	kJ/mol	Joback Method
hf	-85.59	kJ/mol	Joback Method
hfus	15.48	kJ/mol	Joback Method
hvap	33.50	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.460		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
tb	390.30	K	Joback Method
tc	572.19	K	Joback Method
tf	180.72	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.31	J/mol×K	390.30	Joback Method
cpg	200.40	J/mol×K	420.61	Joback Method
cpg	210.98	J/mol×K	450.93	Joback Method
cpg	221.08	J/mol×K	481.24	Joback Method
cpg	230.71	J/mol×K	511.56	Joback Method
cpg	239.91	J/mol×K	541.87	Joback Method
cpg	248.68	J/mol×K	572.19	Joback Method
dvisc	0.0033615	Pa×s	180.72	Joback Method
dvisc	0.0013186	Pa×s	215.65	Joback Method

dvisc	0.0006714	Pa×s	250.58	Joback Method
dvisc	0.0004033	Pa×s	285.51	Joback Method
dvisc	0.0002707	Pa×s	320.44	Joback Method
dvisc	0.0001965	Pa×s	355.37	Joback Method
dvisc	0.0001511	Pa×s	390.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61463283&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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