

1-Butene, 1-ethoxy-3-methyl-, (E)

Inchi:	InChI=1S/C7H14O/c1-4-8-6-5-7(2)3/h5-7H,4H2,1-3H3/b6-5+
InchiKey:	KLKHJTPIDMZMBB-AATRIKPKSA-N
Formula:	C7H14O
SMILES:	CCOC=CC(C)C
Mol. weight [g/mol]:	114.19
CAS:	16969-18-9

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
mvol	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	m ³ /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	Paxs	170.80	Joback Method
dvisc	0.0021300	Paxs	206.62	Joback Method

dvisc	0.0009661	Paxs	242.43	Joback Method
dvisc	0.0005371	Paxs	278.25	Joback Method
dvisc	0.0003414	Paxs	314.07	Joback Method
dvisc	0.0002381	Paxs	349.88	Joback Method
dvisc	0.0001775	Paxs	385.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16969189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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