

1,3-Butadiene, 1-ethoxy-, (E)

Inchi:	InChI=1S/C6H10O/c1-3-5-6-7-4-2/h3,5-6H,1,4H2,2H3/b6-5+
InchiKey:	LDVKFLIDEBQMNX-AATRIKPKSA-N
Formula:	C6H10O
SMILES:	C=CC=COCC
Mol. weight [g/mol]:	98.14
CAS:	19774-34-6

Physical Properties

Property code	Value	Unit	Source
gf	62.70	kJ/mol	Joback Method
hf	-56.74	kJ/mol	Joback Method
hfus	11.41	kJ/mol	Joback Method
hvap	30.65	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.723		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	359.94	K	Joback Method
tc	536.95	K	Joback Method
tf	172.77	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.18	J/mol×K	359.94	Joback Method
cpg	163.52	J/mol×K	389.44	Joback Method
cpg	172.49	J/mol×K	418.94	Joback Method
cpg	181.09	J/mol×K	448.44	Joback Method
cpg	189.33	J/mol×K	477.94	Joback Method
cpg	197.23	J/mol×K	507.44	Joback Method
cpg	204.80	J/mol×K	536.95	Joback Method
dvisc	0.0026699	Pa×s	172.77	Joback Method
dvisc	0.0011945	Pa×s	203.97	Joback Method

dvisc	0.0006615	Pa×s	235.16	Joback Method
dvisc	0.0004208	Pa×s	266.36	Joback Method
dvisc	0.0002943	Pa×s	297.55	Joback Method
dvisc	0.0002202	Pa×s	328.75	Joback Method
dvisc	0.0001733	Pa×s	359.94	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=C19774346&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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