

trans-1-Ethoxy-1-butene

Other names:	1-Butenyl ethyl ether
Inchi:	InChI=1S/C6H12O/c1-3-5-6-7-4-2/h5-6H,3-4H2,1-2H3/b6-5+
InchiKey:	AQTYNINXYJFSHD-AATRIKPKSA-N
Formula:	C6H12O
SMILES:	CCC=COCC
Mol. weight [g/mol]:	100.16

Physical Properties

Property code	Value	Unit	Source
gf	-25.14	kJ/mol	Joback Method
hf	-182.17	kJ/mol	Joback Method
hfus	12.69	kJ/mol	Joback Method
hvap	31.32	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.947		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	687.00		NIST Webbook
tb	363.26	K	Joback Method
tc	536.57	K	Joback Method
tf	174.53	K	Joback Method
vc	0.369	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.70	J/molxK	363.26	Joback Method
cpg	214.08	J/molxK	507.68	Joback Method
cpg	205.48	J/molxK	478.80	Joback Method
cpg	196.56	J/molxK	449.91	Joback Method
cpg	187.29	J/molxK	421.03	Joback Method
cpg	177.67	J/molxK	392.14	Joback Method
cpg	222.34	J/molxK	536.57	Joback Method
dvisc	0.0001803	Paxs	363.26	Joback Method

dvisc	0.0002325	Paxs	331.80	Joback Method
dvisc	0.0003162	Paxs	300.35	Joback Method
dvisc	0.0004620	Paxs	268.89	Joback Method
dvisc	0.0007464	Paxs	237.44	Joback Method
dvisc	0.0013962	Paxs	205.99	Joback Method
dvisc	0.0032729	Paxs	174.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U139439&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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