1-ethoxy-2,4-hexadiene

Other names: 2,4-Hexadiene, 1-ethoxy
Inchi: InChI=1S/C8H14O/c1-3-5-6-7-8-9-4-2/h3,5-7H,4,8H2,1-2H3/b5-3+,7-6-
InchiKey: UNHPVHFNZXRVNU-WZWXSLMZSA-N
Formula: C8H14O
SMILES: CC=CC=CCOCC
Mol. weight [g/mol]: 126.20

Physical Properties

Property code	Value	Unit	Source
gf	71.92	kJ/mol	Joback Method
hf	-106.23	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	35.73	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	2.155		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	940.00		NIST Webbook
tb	413.18	K	Joback Method
tc	593.96	K	Joback Method
tf	191.99	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.62	J/mol×K	413.18	Joback Method
cpg	239.92	J/mol×K	443.31	Joback Method
cpg	251.66	J/mol×K	473.44	Joback Method
cpg	262.87	J/mol×K	503.57	Joback Method
cpg	273.58	J/mol×K	533.70	Joback Method
cpg	283.79	J/mol×K	563.83	Joback Method
cpg	293.54	J/mol×K	593.96	Joback Method
dvisc	0.0036057	Pa×s	191.99	Joback Method

dvisc	0.0013874	Pa×s	228.86	Joback Method
dvisc	0.0006959	Pa×s	265.72	Joback Method
dvisc	0.0004129	Pa×s	302.59	Joback Method
dvisc	0.0002744	Pa×s	339.45	Joback Method
dvisc	0.0001976	Pa×s	376.32	Joback Method
dvisc	0.0001509	Pa×s	413.18	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=U365965&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume