

2-ethoxy-3,5-hexadiene

Other names:	3,5-Hexadiene, 2-ethoxy
Inchi:	InChI=1S/C8H14O/c1-4-6-7-8(3)9-5-2/h4,6-8H,1,5H2,2-3H3/b7-6+
InchiKey:	IXTXFMUQEVEFFL-VOTSOKGWSA-N
Formula:	C8H14O
SMILES:	C=CC=CC(C)OCC
Mol. weight [g/mol]:	126.20

Physical Properties

Property code	Value	Unit	Source
gf	77.10	kJ/mol	Joback Method
hf	-103.30	kJ/mol	Joback Method
hfus	13.06	kJ/mol	Joback Method
hvap	34.71	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.154		Crippen Method
mcpvol	120.850	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	846.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	850.00		NIST Webbook
tb	405.26	K	Joback Method
tc	584.99	K	Joback Method
tf	180.31	K	Joback Method
vc	0.457	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.43	J/mol×K	405.26	Joback Method
cpg	239.75	J/mol×K	435.22	Joback Method
cpg	251.55	J/mol×K	465.17	Joback Method
cpg	262.85	J/mol×K	495.13	Joback Method
cpg	273.66	J/mol×K	525.08	Joback Method
cpg	284.00	J/mol×K	555.04	Joback Method

cpg	293.89	J/molxK	584.99	Joback Method
dvisc	0.0056730	Paxs	180.31	Joback Method
dvisc	0.0019202	Paxs	217.80	Joback Method
dvisc	0.0008935	Paxs	255.29	Joback Method
dvisc	0.0005057	Paxs	292.78	Joback Method
dvisc	0.0003257	Paxs	330.28	Joback Method
dvisc	0.0002295	Paxs	367.77	Joback Method
dvisc	0.0001725	Paxs	405.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U365966&Units=SI

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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