3-Hexene, 1-(1-methoxyethoxy)-, (Z)-

Other names: Methyl (Z)-3-hexenyl acetal
Inchi: InChI=1S/C9H18O2/c1-4-5-6-7-8-11-9(2)10-3/h5-6,9H,4,7-8H2,1-3H3/b6-5-
InchiKey: BFFNMPRAXYAFMS-WAYWQWQTSA-N
Formula: C9H18O2
SMILES: CCC=CCCOC(C)OC
Mol. weight [g/mol]: 158.24
CAS: 54340-96-4

Physical Properties

Property code	Value	Unit	Source
gf	-107.32	kJ/mol	Joback Method
hf	-381.59	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	40.02	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.352		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1267.00		NIST Webbook
tb	453.88	K	Joback Method
tc	628.53	K	Joback Method
tf	215.57	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.00	J/mol×K	453.88	Joback Method
cpg	372.71	J/mol×K	599.42	Joback Method
cpg	360.91	J/mol×K	570.31	Joback Method
cpg	348.64	J/mol×K	541.21	Joback Method

cpg	335.91	J/mol×K	512.10	Joback Method
cpg	322.69	J/mol×K	482.99	Joback Method
cpg	384.06	J/mol×K	628.53	Joback Method
dvisc	0.0001447	Pa×s	453.88	Joback Method
dvisc	0.0001952	Pa×s	414.16	Joback Method
dvisc	0.0002805	Pa×s	374.44	Joback Method
dvisc	0.0004394	Pa×s	334.73	Joback Method
dvisc	0.0007766	Pa×s	295.01	Joback Method
dvisc	0.0016389	Pa×s	255.29	Joback Method
dvisc	0.0045543	Pa×s	215.57	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C54340964&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume