E-1-Methoxy-3-hexene

Other names: (3E)-1-Methoxy-3-hexene
(E)-3-Hexenyl methyl ether
trans-1-Methoxy-3-hexene
Inchi: InChI=1S/C7H14O/c1-3-4-5-6-7-8-2/h4-5H,3,6-7H2,1-2H3/b5-4+
InchiKey: KUPODEXLSGEWFR-SNAWJCMRSA-N
Formula: C7H14O
SMILES: CCC=CCCOC
Mol. weight [g/mol]: 114.19
CAS: 121441-40-5

Physical Properties

Property code	Value	Unit	Source
gf	-16.72	kJ/mol	Joback Method
hf	-202.81	kJ/mol	Joback Method
hfus	15.28	kJ/mol	Joback Method
hvap	33.54	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.989		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	810.00		NIST Webbook
rinpol	810.00		NIST Webbook
ripol	974.00		NIST Webbook
tb	386.14	K	Joback Method
tc	558.99	K	Joback Method
tf	185.80	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.98	J/mol×K	386.14	Joback Method
cpg	256.48	J/mol×K	530.18	Joback Method
cpg	246.77	J/mol×K	501.37	Joback Method

cpg	236.68	J/mol×K	472.57	Joback Method
cpg	226.18	J/mol×K	443.76	Joback Method
cpg	215.29	J/mol×K	414.95	Joback Method
cpg	265.82	J/mol×K	558.99	Joback Method
dvisc	0.0001834	Pa×s	386.14	Joback Method
dvisc	0.0002383	Pa×s	352.75	Joback Method
dvisc	0.0003271	Pa×s	319.36	Joback Method
dvisc	0.0004833	Pa×s	285.97	Joback Method
dvisc	0.0007918	Pa×s	252.58	Joback Method
dvisc	0.0015077	Pa×s	219.19	Joback Method
dvisc	0.0036187	Pa×s	185.80	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=C121441405&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