3-Hexene, 3-methoxy-2-methyl-, (Z)-

Inchi: InChI=1S/C8H16O/c1-5-6-8(9-4)7(2)3/h6-7H,5H2,1-4H3/b8-6-
InchiKey: KLLLUNXXSVCGMP-VURMDHGXSA-N
Formula: C8H16O
SMILES: CCC=C(OC)C(C)C
Mol. weight [g/mol]: 128.21
CAS: 66017-21-8

Physical Properties

Property code	Value	Unit	Source
gf	-19.29	kJ/mol	Joback Method
hf	-238.52	kJ/mol	Joback Method
hfus	13.03	kJ/mol	Joback Method
hvap	35.46	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.583		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	408.46	K	Joback Method
tc	587.94	K	Joback Method
tf	168.11	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.59	J/mol×K	408.46	Joback Method
cpg	255.70	J/mol×K	438.37	Joback Method
cpg	268.30	J/mol×K	468.29	Joback Method
cpg	280.40	J/mol×K	498.20	Joback Method
cpg	292.01	J/mol×K	528.12	Joback Method
cpg	303.14	J/mol×K	558.03	Joback Method
cpg	313.81	J/mol×K	587.94	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=C66017218&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume