3-Hexene, 3-methoxy-2,5-dimethyl-, (E)-

Inchi: InChI=1S/C9H18O/c1-7(2)6-9(10-5)8(3)4/h6-8H,1-5H3/b9-6+
InchiKey: PYPPCCYSBRCXAF-RMKNXTFCSA-N
Formula: C9H18O
SMILES: COC(=CC(C)C)C(C)C
Mol. weight [g/mol]: 142.24
CAS: 66017-23-0

Physical Properties

Property code	Value	Unit	Source
gf	-13.31	kJ/mol	Joback Method
hf	-264.44	kJ/mol	Joback Method
hfus	12.10	kJ/mol	Joback Method
hvap	37.30	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.829		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
tb	430.90	K	Joback Method
tc	613.21	K	Joback Method
tf	164.38	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.59	J/mol×K	430.90	Joback Method
cpg	298.22	J/mol×K	461.28	Joback Method
cpg	312.26	J/mol×K	491.67	Joback Method
cpg	325.72	J/mol×K	522.05	Joback Method
cpg	338.60	J/mol×K	552.44	Joback Method
cpg	350.94	J/mol×K	582.82	Joback Method
cpg	362.73	J/mol×K	613.21	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=C66017230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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