

2,5-Dimethyl-3-methoxy-hexene

Inchi:	InChI=1S/C9H18O/c1-7(2)6-9(10-5)8(3)4/h7H,6H2,1-5H3
InchiKey:	RNXMYQBHWTXSGP-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	COC(CC(C)C)=C(C)C
Mol. weight [g/mol]:	142.24
CAS:	66017-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-19.42	kJ/mol	Joback Method
hf	-268.95	kJ/mol	Joback Method
hfus	14.31	kJ/mol	Joback Method
hvap	37.77	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.973		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
tb	431.22	K	Joback Method
tc	612.90	K	Joback Method
tf	165.42	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.50	J/mol×K	431.22	Joback Method
cpg	297.97	J/mol×K	461.50	Joback Method
cpg	311.84	J/mol×K	491.78	Joback Method
cpg	325.15	J/mol×K	522.06	Joback Method
cpg	337.90	J/mol×K	552.34	Joback Method
cpg	350.11	J/mol×K	582.62	Joback Method
cpg	361.80	J/mol×K	612.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C66017229&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

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