

# Hexane, 3-methoxy-

Inchi:	InChI=1S/C7H16O/c1-4-6-7(5-2)8-3/h7H,4-6H2,1-3H3
InchiKey:	QNJRNZBXNCPKHQ-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCC(CC)OC
Mol. weight [g/mol]:	116.20
CAS:	54658-01-4

## Physical Properties

Property code	Value	Unit	Source
gf	-99.38	kJ/mol	Joback Method
hf	-325.31	kJ/mol	Joback Method
hfus	11.55	kJ/mol	Joback Method
hvap	33.20	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.212		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	381.54	K	Joback Method
tc	549.69	K	Joback Method
tf	175.88	K	Joback Method
vc	0.440	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.33	J/molxK	381.54	Joback Method
cpg	230.17	J/molxK	409.57	Joback Method
cpg	241.65	J/molxK	437.59	Joback Method
cpg	252.77	J/molxK	465.62	Joback Method
cpg	263.53	J/molxK	493.64	Joback Method
cpg	273.94	J/molxK	521.67	Joback Method
cpg	284.00	J/molxK	549.69	Joback Method
dvisc	0.0068890	Paxs	175.88	Joback Method
dvisc	0.0024170	Paxs	210.16	Joback Method

dvisc	0.0011375	Paxs	244.43	Joback Method
dvisc	0.0006444	Paxs	278.71	Joback Method
dvisc	0.0004135	Paxs	312.99	Joback Method
dvisc	0.0002896	Paxs	347.26	Joback Method
dvisc	0.0002162	Paxs	381.54	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C54658014&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54658014&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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