

# Hexadecane, 3-octyl

<b>Inchi:</b>	InChI=1S/C24H50/c1-4-7-9-11-13-14-15-16-17-19-21-23-24(6-3)22-20-18-12-10-8-5-2/h
<b>InchiKey:</b>	PMMXWTWKCTZRRQ-UHFFFAOYSA-N
<b>Formula:</b>	C24H50
<b>SMILES:</b>	CCCCCCCCCCCC(C)CCCCCCC
<b>Mol. weight [g/mol]:</b>	338.65

## Physical Properties

Property code	Value	Unit	Source
gf	148.76	kJ/mol	Joback Method
hf	-543.97	kJ/mol	Joback Method
hfus	54.39	kJ/mol	Joback Method
hvap	68.63	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	9.464		Crippen Method
mvol	349.020	ml/mol	McGowan Method
pc	809.83	kPa	Joback Method
rinpol	2315.00		NIST Webbook
rinpol	2315.00		NIST Webbook
tb	748.08	K	Joback Method
tc	918.22	K	Joback Method
tf	345.24	K	Joback Method
vc	1.373	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.86	J/molxK	748.08	Joback Method
cpg	1192.43	J/molxK	889.86	Joback Method
cpg	1173.45	J/molxK	861.51	Joback Method
cpg	1153.54	J/molxK	833.15	Joback Method
cpg	1132.66	J/molxK	804.79	Joback Method
cpg	1110.78	J/molxK	776.44	Joback Method
cpg	1210.52	J/molxK	918.22	Joback Method
dvisc	0.0000532	Paxs	748.08	Joback Method

dvisc	0.0000751	Paxs	680.94	Joback Method
dvisc	0.0001142	Paxs	613.80	Joback Method
dvisc	0.0001924	Paxs	546.66	Joback Method
dvisc	0.0003752	Paxs	479.52	Joback Method
dvisc	0.0009096	Paxs	412.38	Joback Method
dvisc	0.0031119	Paxs	345.24	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=R47657&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R47657&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>rinpol:</b>	Non-polar retention indices
<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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