

# Hexadecane, 6-butyl

Inchi:	InChI=1S/C20H42/c1-4-7-10-11-12-13-14-16-19-20(17-9-6-3)18-15-8-5-2/h20H,4-19H2,1
InchiKey:	UOERRVFDJDOEBT-UHFFFAOYSA-N
Formula:	C20H42
SMILES:	CCCCCCCCCCC(CCCC)CCCC
Mol. weight [g/mol]:	282.55

## Physical Properties

Property code	Value	Unit	Source
gf	115.08	kJ/mol	Joback Method
hf	-461.41	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	59.73	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.904		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
pc	1020.73	kPa	Joback Method
rinpol	1887.00		NIST Webbook
rinpol	1887.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	656.56	K	Joback Method
tc	818.58	K	Joback Method
tf	300.16	K	Joback Method
vc	1.149	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.82	J/molxK	656.56	Joback Method
cpg	862.00	J/molxK	683.56	Joback Method
cpg	882.29	J/molxK	710.57	Joback Method
cpg	901.73	J/molxK	737.57	Joback Method
cpg	920.35	J/molxK	764.58	Joback Method
cpg	938.17	J/molxK	791.58	Joback Method

cpg	955.21	J/mol×K	818.58	Joback Method
dvisc	0.0051032	Paxs	300.16	Joback Method
dvisc	0.0014944	Paxs	359.56	Joback Method
dvisc	0.0006199	Paxs	418.96	Joback Method
dvisc	0.0003200	Paxs	478.36	Joback Method
dvisc	0.0001911	Paxs	537.76	Joback Method
dvisc	0.0001265	Paxs	597.16	Joback Method
dvisc	0.0000902	Paxs	656.56	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R8627&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R8627&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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