

# Benzene, 1-butyl-2-hexyl

<b>Inchi:</b>	InChI=1S/C16H26/c1-3-5-7-8-12-16-14-10-9-13-15(16)11-6-4-2/h9-10,13-14H,3-8,11-12H
<b>InchiKey:</b>	QZSAPOQAHFFCHS-UHFFFAOYSA-N
<b>Formula:</b>	C16H26
<b>SMILES:</b>	CCCCCc1ccccc1CCCC
<b>Mol. weight [g/mol]:</b>	218.38

## Physical Properties

Property code	Value	Unit	Source
gf	186.62	kJ/mol	Joback Method
hf	-148.51	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	54.15	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.152		Crippen Method
mvol	212.540	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	597.14	K	Joback Method
tc	787.38	K	Joback Method
tf	309.02	K	Joback Method
vc	0.824	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.23	J/molxK	597.14	Joback Method
cpg	630.29	J/molxK	755.67	Joback Method
cpg	615.03	J/molxK	723.97	Joback Method
cpg	598.94	J/molxK	692.26	Joback Method
cpg	581.96	J/molxK	660.55	Joback Method
cpg	564.07	J/molxK	628.85	Joback Method
cpg	644.73	J/molxK	787.38	Joback Method
dvisc	0.0001482	Paxs	597.14	Joback Method

dvisc	0.0001929	Paxs	549.12	Joback Method
dvisc	0.0002641	Paxs	501.10	Joback Method
dvisc	0.0003863	Paxs	453.08	Joback Method
dvisc	0.0006186	Paxs	405.06	Joback Method
dvisc	0.0011242	Paxs	357.04	Joback Method
dvisc	0.0024600	Paxs	309.02	Joback Method

## Sources

<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>
<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=R13624&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R13624&amp;Units=SI</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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