

# Benzene, 1-butyl-4-propyl

<b>Inchi:</b>	InChI=1S/C13H20/c1-3-5-7-13-10-8-12(6-4-2)9-11-13/h8-11H,3-7H2,1-2H3
<b>InchiKey:</b>	YKYP CWLDEQIAAX-UHFFFAOYSA-N
<b>Formula:</b>	C13H20
<b>SMILES:</b>	CCCCc1ccc(CCC)cc1
<b>Mol. weight [g/mol]:</b>	176.30

## Physical Properties

Property code	Value	Unit	Source
gf	161.36	kJ/mol	Joback Method
hf	-86.59	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.982		Crippen Method
mvol	170.270	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
ripol	1535.00		NIST Webbook
tb	528.50	K	Joback Method
tc	726.20	K	Joback Method
tf	275.21	K	Joback Method
vc	0.655	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.45	J/molxK	528.50	Joback Method
cpg	471.14	J/molxK	693.25	Joback Method
cpg	457.24	J/molxK	660.30	Joback Method
cpg	442.55	J/molxK	627.35	Joback Method
cpg	427.04	J/molxK	594.40	Joback Method
cpg	410.68	J/molxK	561.45	Joback Method
cpg	484.29	J/molxK	726.20	Joback Method
dvisc	0.0001884	Paxs	528.50	Joback Method
dvisc	0.0002417	Paxs	486.28	Joback Method

dvisc	0.0003251	Paxs	444.07	Joback Method
dvisc	0.0004654	Paxs	401.86	Joback Method
dvisc	0.0007248	Paxs	359.64	Joback Method
dvisc	0.0012700	Paxs	317.42	Joback Method
dvisc	0.0026431	Paxs	275.21	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=R12583&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R12583&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>ripol:</b>	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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