

# 2-(3-Hexyl)phenol

<b>Inchi:</b>	InChI=1S/C12H18O/c1-3-7-10(4-2)11-8-5-6-9-12(11)13/h5-6,8-10,13H,3-4,7H2,1-2H3
<b>InchiKey:</b>	UVOWWKIXBXXDMK-UHFFFAOYSA-N
<b>Formula:</b>	C12H18O
<b>SMILES:</b>	CCCC(CC)c1ccccc1O
<b>Mol. weight [g/mol]:</b>	178.27
<b>CAS:</b>	91763-74-5

## Physical Properties

Property code	Value	Unit	Source
gf	5.51	kJ/mol	Joback Method
hf	-237.07	kJ/mol	Joback Method
hfus	23.14	kJ/mol	Joback Method
hvap	57.21	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.686		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	580.82	K	Joback Method
tc	796.40	K	Joback Method
tf	348.14	K	Joback Method
vc	0.559	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.71	J/molxK	580.82	Joback Method
cpg	421.37	J/molxK	616.75	Joback Method
cpg	436.03	J/molxK	652.68	Joback Method
cpg	449.78	J/molxK	688.61	Joback Method
cpg	462.71	J/molxK	724.54	Joback Method
cpg	474.88	J/molxK	760.47	Joback Method
cpg	486.39	J/molxK	796.40	Joback Method
dvisc	0.0036794	Paxs	348.14	Joback Method
dvisc	0.0011551	Paxs	386.92	Joback Method

dvisc	0.0004478	Paxs	425.70	Joback Method
dvisc	0.0002034	Paxs	464.48	Joback Method
dvisc	0.0001043	Paxs	503.26	Joback Method
dvisc	0.0000589	Paxs	542.04	Joback Method
dvisc	0.0000359	Paxs	580.82	Joback Method

## Sources

<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=C91763745&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C91763745&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>

## 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>mccvol:</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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