

# Phenol, 4-(1-propylhexyl)

<b>Inchi:</b>	InChI=1S/C15H24O/c1-3-5-6-8-13(7-4-2)14-9-11-15(16)12-10-14/h9-13,16H,3-8H2,1-2H
<b>InchiKey:</b>	GPCIEYNIMWVQBI-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CCCCC(CCC)c1ccc(O)cc1
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	30.77	kJ/mol	Joback Method
hf	-298.99	kJ/mol	Joback Method
hfus	30.91	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.856		Crippen Method
mvol	204.320	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	649.46	K	Joback Method
tc	854.96	K	Joback Method
tf	381.95	K	Joback Method
vc	0.728	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.07	J/molxK	649.46	Joback Method
cpg	575.21	J/molxK	683.71	Joback Method
cpg	591.38	J/molxK	717.96	Joback Method
cpg	606.65	J/molxK	752.21	Joback Method
cpg	621.10	J/molxK	786.46	Joback Method
cpg	634.82	J/molxK	820.71	Joback Method
cpg	647.87	J/molxK	854.96	Joback Method
dvisc	0.0018851	Paxs	381.95	Joback Method

dvisc	0.0005800	Paxs	426.53	Joback Method
dvisc	0.0002231	Paxs	471.12	Joback Method
dvisc	0.0001012	Paxs	515.71	Joback Method
dvisc	0.0000521	Paxs	560.29	Joback Method
dvisc	0.0000295	Paxs	604.88	Joback Method
dvisc	0.0000181	Paxs	649.46	Joback Method

## Sources

<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=R592906&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R592906&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>

## 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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