

# Phenol, 4-(1-ethyl-1-methylhexyl)

<b>Inchi:</b>	InChI=1S/C15H24O/c1-4-6-7-12-15(3,5-2)13-8-10-14(16)11-9-13/h8-11,16H,4-7,12H2,1-
<b>InchiKey:</b>	QQKQQJZGUCFUPP-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CCCCC(C)(CC)c1ccc(O)cc1
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	36.05	kJ/mol	Joback Method
hf	-302.46	kJ/mol	Joback Method
hfus	27.02	kJ/mol	Joback Method
hvap	62.98	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.640		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
tb	646.67	K	Joback Method
tc	859.37	K	Joback Method
tf	399.37	K	Joback Method
vc	0.723	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.46	J/molxK	646.67	Joback Method
cpg	577.98	J/molxK	682.12	Joback Method
cpg	594.40	J/molxK	717.57	Joback Method
cpg	609.82	J/molxK	753.02	Joback Method
cpg	624.36	J/molxK	788.47	Joback Method

cpg	638.12	J/mol×K	823.92	Joback Method
cpg	651.21	J/mol×K	859.37	Joback Method
dvisc	0.0012837	Paxs	399.37	Joback Method
dvisc	0.0004464	Paxs	440.59	Joback Method
dvisc	0.0001860	Paxs	481.80	Joback Method
dvisc	0.0000889	Paxs	523.02	Joback Method
dvisc	0.0000474	Paxs	564.24	Joback Method
dvisc	0.0000275	Paxs	605.45	Joback Method
dvisc	0.0000171	Paxs	646.67	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=R591983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R591983&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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