

# Phenol, 4-(1-ethyl-1,3-dimethylpentyl), diastereomer # 1

Inchi:	InChI=1S/C15H24O/c1-5-12(3)11-15(4,6-2)13-7-9-14(16)10-8-13/h7-10,12,16H,5-6,11H2
InchiKey:	RYIHVIPUIXFRNI-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CCC(C)CC(C)(CC)c1ccc(O)cc1
Mol. weight [g/mol]:	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	33.61	kJ/mol	Joback Method
hf	-307.74	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.496		Crippen Method
mvol	204.320	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	1710.00		NIST Webbook
tb	646.23	K	Joback Method
tc	863.09	K	Joback Method
tf	384.37	K	Joback Method
vc	0.717	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.90	J/molxK	646.23	Joback Method
cpg	640.01	J/molxK	826.95	Joback Method
cpg	626.04	J/molxK	790.81	Joback Method
cpg	611.26	J/molxK	754.66	Joback Method
cpg	595.55	J/molxK	718.52	Joback Method
cpg	578.81	J/molxK	682.37	Joback Method
cpg	653.27	J/molxK	863.09	Joback Method
dvisc	0.0000159	Paxs	646.23	Joback Method
dvisc	0.0000265	Paxs	602.59	Joback Method

dvisc	0.0000478	Paxs	558.94	Joback Method
dvisc	0.0000953	Paxs	515.30	Joback Method
dvisc	0.0002155	Paxs	471.66	Joback Method
dvisc	0.0005760	Paxs	428.01	Joback Method
dvisc	0.0019247	Paxs	384.37	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=R592659&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R592659&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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