

# Phenol, 4-(2-ethyl-1,1-dimethylbutyl)

<b>Inchi:</b>	InChI=1S/C14H22O/c1-5-11(6-2)14(3,4)12-7-9-13(15)10-8-12/h7-11,15H,5-6H2,1-4H3
<b>InchiKey:</b>	KDAVNYSBTBWHQK-UHFFFAOYSA-N
<b>Formula:</b>	C14H22O
<b>SMILES:</b>	CCC(CC)C(C)(C)c1ccc(O)cc1
<b>Mol. weight [g/mol]:</b>	206.32

## Physical Properties

Property code	Value	Unit	Source
gf	25.19	kJ/mol	Joback Method
hf	-287.10	kJ/mol	Joback Method
hfus	20.90	kJ/mol	Joback Method
hvap	60.36	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	4.106		Crippen Method
mvol	190.230	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1729.00		NIST Webbook
rinpol	1729.00		NIST Webbook
tb	623.35	K	Joback Method
tc	844.06	K	Joback Method
tf	373.10	K	Joback Method
vc	0.660	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.87	J/molxK	623.35	Joback Method
cpg	585.91	J/molxK	807.27	Joback Method
cpg	572.41	J/molxK	770.49	Joback Method
cpg	558.07	J/molxK	733.70	Joback Method
cpg	542.77	J/molxK	696.92	Joback Method
cpg	526.41	J/molxK	660.13	Joback Method
cpg	598.69	J/molxK	844.06	Joback Method
dvisc	0.0000203	Paxs	623.35	Joback Method

dvisc	0.0000338	Paxs	581.64	Joback Method
dvisc	0.0000611	Paxs	539.93	Joback Method
dvisc	0.0001219	Paxs	498.22	Joback Method
dvisc	0.0002758	Paxs	456.52	Joback Method
dvisc	0.0007356	Paxs	414.81	Joback Method
dvisc	0.0024425	Paxs	373.10	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=R592966&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R592966&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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