

# Phenol, 4-(1-ethyl-2,3,3-trimethylbutyl), diastereomer # 1

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

## Physical Properties

Property code	Value	Unit	Source
gf	31.17	kJ/mol	Joback Method
hf	-313.02	kJ/mol	Joback Method
hfus	19.97	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.568		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1733.00		NIST Webbook
tb	645.79	K	Joback Method
tc	866.98	K	Joback Method
tf	369.37	K	Joback Method
vc	0.711	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.35	J/molxK	645.79	Joback Method
cpg	579.65	J/molxK	682.65	Joback Method
cpg	596.74	J/molxK	719.52	Joback Method
cpg	612.74	J/molxK	756.38	Joback Method
cpg	627.76	J/molxK	793.25	Joback Method
cpg	641.94	J/molxK	830.11	Joback Method
cpg	655.38	J/molxK	866.98	Joback Method
dvisc	0.0030151	Paxs	369.37	Joback Method
dvisc	0.0007611	Paxs	415.44	Joback Method

dvisc	0.0002529	Paxs	461.51	Joback Method
dvisc	0.0001026	Paxs	507.58	Joback Method
dvisc	0.0000484	Paxs	553.65	Joback Method
dvisc	0.0000256	Paxs	599.72	Joback Method
dvisc	0.0000148	Paxs	645.79	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=R592699&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R592699&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>

## 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>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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