

# Phenol, 4-(1,2-diethyl-3-methylbutyl), diastereomer # 2

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

## Physical Properties

Property code	Value	Unit	Source
gf	25.89	kJ/mol	Joback Method
hf	-309.55	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	63.11	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.568		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1759.00		NIST Webbook
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tb	648.58	K	Joback Method
tc	861.97	K	Joback Method
tf	351.95	K	Joback Method
vc	0.716	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.96	J/molxK	648.58	Joback Method
cpg	638.52	J/molxK	826.40	Joback Method
cpg	624.40	J/molxK	790.84	Joback Method
cpg	609.47	J/molxK	755.27	Joback Method
cpg	593.65	J/molxK	719.71	Joback Method
cpg	576.84	J/molxK	684.14	Joback Method
cpg	651.91	J/molxK	861.97	Joback Method
dvisc	0.0000157	Paxs	648.58	Joback Method

dvisc	0.0000275	Paxs	599.14	Joback Method
dvisc	0.0000530	Paxs	549.70	Joback Method
dvisc	0.0001165	Paxs	500.26	Joback Method
dvisc	0.0003045	Paxs	450.83	Joback Method
dvisc	0.0010084	Paxs	401.39	Joback Method
dvisc	0.0046742	Paxs	351.95	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R592520&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R592520&amp;Units=SI</a>
<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>

## 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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