

# 1-Naphthol, isoBOC

<b>Inchi:</b>	InChI=1S/C15H16O3/c1-11(2)10-17-15(16)18-14-9-5-7-12-6-3-4-8-13(12)14/h3-9,11H,10
<b>InchiKey:</b>	UBAMHKZYHOHSLK-UHFFFAOYSA-N
<b>Formula:</b>	C15H16O3
<b>SMILES:</b>	CC(C)COC(=O)Oc1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	244.29

## Physical Properties

Property code	Value	Unit	Source
gf	-56.51	kJ/mol	Joback Method
hf	-319.10	kJ/mol	Joback Method
hfus	25.73	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.011		Crippen Method
mcvol	192.300	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rmpol	1895.00		NIST Webbook
tb	691.51	K	Joback Method
tc	915.00	K	Joback Method
tf	409.84	K	Joback Method
vc	0.726	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.44	J/molxK	691.51	Joback Method
cpg	576.70	J/molxK	877.75	Joback Method
cpg	565.55	J/molxK	840.50	Joback Method
cpg	553.49	J/molxK	803.26	Joback Method
cpg	540.48	J/molxK	766.01	Joback Method
cpg	526.47	J/molxK	728.76	Joback Method
cpg	586.98	J/molxK	915.00	Joback Method
dvisc	0.0001743	Paxs	691.51	Joback Method
dvisc	0.0002138	Paxs	644.57	Joback Method

dvisc	0.0002706	Paxs	597.62	Joback Method
dvisc	0.0003567	Paxs	550.67	Joback Method
dvisc	0.0004950	Paxs	503.73	Joback Method
dvisc	0.0007346	Paxs	456.79	Joback Method
dvisc	0.0011936	Paxs	409.84	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=R234878&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R234878&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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