

# Hydroquinone, isoBOC

<b>Inchi:</b>	InChI=1S/C16H22O6/c1-11(2)9-19-15(17)21-13-5-7-14(8-6-13)22-16(18)20-10-12(3)4/h5
<b>InchiKey:</b>	MOURESOROCNEAM-UHFFFAOYSA-N
<b>Formula:</b>	C16H22O6
<b>SMILES:</b>	CC(C)COC(=O)Oc1ccc(OC(=O)OCC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	310.34

## Physical Properties

Property code	Value	Unit	Source
gf	-496.10	kJ/mol	Joback Method
hf	-913.11	kJ/mol	Joback Method
hfus	31.75	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.029		Crippen Method
mvol	239.160	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook
tb	793.68	K	Joback Method
tc	999.55	K	Joback Method
tf	467.80	K	Joback Method
vc	0.895	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.25	J/molxK	793.68	Joback Method
cpg	767.32	J/molxK	965.24	Joback Method
cpg	757.23	J/molxK	930.93	Joback Method
cpg	745.96	J/molxK	896.62	Joback Method
cpg	733.54	J/molxK	862.30	Joback Method
cpg	719.96	J/molxK	827.99	Joback Method
cpg	776.22	J/molxK	999.55	Joback Method
dvisc	0.0000457	Paxs	793.68	Joback Method

dvisc	0.0000595	Paxs	739.37	Joback Method
dvisc	0.0000808	Paxs	685.05	Joback Method
dvisc	0.0001156	Paxs	630.74	Joback Method
dvisc	0.0001772	Paxs	576.43	Joback Method
dvisc	0.0002966	Paxs	522.11	Joback Method
dvisc	0.0005597	Paxs	467.80	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=R235282&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R235282&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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