

# isotorquatone

<b>Inchi:</b>	InChI=1S/C16H24O4/c1-8-9(2)13(17)12-15(19-6)10(3)14(18-5)11(4)16(12)20-7/h9H,8H2
<b>InchiKey:</b>	NPBLAHCDLPLESG-UHFFFAOYSA-N
<b>Formula:</b>	C16H24O4
<b>SMILES:</b>	CCC(C)C(=O)c1c(OC)c(C)c(OC)c(C)c1OC
<b>Mol. weight [g/mol]:</b>	280.36

## Physical Properties

Property code	Value	Unit	Source
gf	-298.26	kJ/mol	Joback Method
hf	-708.91	kJ/mol	Joback Method
hfus	30.93	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.558		Crippen Method
mcvol	231.720	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	1777.00		NIST Webbook
tb	737.75	K	Joback Method
tc	938.11	K	Joback Method
tf	460.72	K	Joback Method
vc	0.877	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.24	J/molxK	737.75	Joback Method
cpg	726.49	J/molxK	904.71	Joback Method
cpg	714.16	J/molxK	871.32	Joback Method
cpg	700.85	J/molxK	837.93	Joback Method
cpg	686.57	J/molxK	804.54	Joback Method
cpg	671.37	J/molxK	771.14	Joback Method
cpg	737.82	J/molxK	938.11	Joback Method
dvisc	0.0000674	Paxs	737.75	Joback Method
dvisc	0.0000826	Paxs	691.58	Joback Method

dvisc	0.0001042	Paxs	645.41	Joback Method
dvisc	0.0001362	Paxs	599.24	Joback Method
dvisc	0.0001862	Paxs	553.06	Joback Method
dvisc	0.0002694	Paxs	506.89	Joback Method
dvisc	0.0004199	Paxs	460.72	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=R301770&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R301770&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>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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