

# 2-Methylresorcinol, isoBOC

<b>Inchi:</b>	InChI=1S/C17H24O6/c1-11(2)9-20-16(18)22-14-7-6-8-15(13(14)5)23-17(19)21-10-12(3)
<b>InchiKey:</b>	SDOMBJYIKTXHBY-UHFFFAOYSA-N
<b>Formula:</b>	C17H24O6
<b>SMILES:</b>	<chem>Cc1c(OC(=O)OCC(C)C)cccc1OC(=O)OCC(C)C</chem>
<b>Mol. weight [g/mol]:</b>	324.37

## Physical Properties

Property code	Value	Unit	Source
gf	-497.31	kJ/mol	Joback Method
hf	-945.22	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	79.39	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.338		Crippen Method
mcvol	253.250	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2105.00		NIST Webbook
tb	821.54	K	Joback Method
tc	1027.28	K	Joback Method
tf	491.59	K	Joback Method
vc	0.952	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.18	J/molxK	821.54	Joback Method
cpg	775.96	J/molxK	855.83	Joback Method
cpg	789.55	J/molxK	890.12	Joback Method
cpg	801.94	J/molxK	924.41	Joback Method
cpg	813.09	J/molxK	958.70	Joback Method
cpg	823.01	J/molxK	992.99	Joback Method
cpg	831.66	J/molxK	1027.28	Joback Method
dvisc	0.0004277	Paxs	491.59	Joback Method
dvisc	0.0002363	Paxs	546.58	Joback Method

dvisc	0.0001455	Paxs	601.57	Joback Method
dvisc	0.0000972	Paxs	656.57	Joback Method
dvisc	0.0000691	Paxs	711.56	Joback Method
dvisc	0.0000516	Paxs	766.55	Joback Method
dvisc	0.0000401	Paxs	821.54	Joback Method

## Sources

<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=R235059&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R235059&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>

## 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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