

# Artedouglasia oxide B

<b>Other names:</b>	B-Artedouglasia oxide
<b>Inchi:</b>	InChI=1S/C15H22O3/c1-6-14(4)10-8-12(17-14)15(5)11(16)7-9-13(2,3)18-15/h6-7,9,12H,
<b>InchiKey:</b>	YDGSUVJUYWCJCE-UCWKZMIHSA-N
<b>Formula:</b>	C15H22O3
<b>SMILES:</b>	C=CC1(C)CCC(C2(C)OC(C)(C)C=CC2=O)O1
<b>Mol. weight [g/mol]:</b>	250.33

## Physical Properties

Property code	Value	Unit	Source
gf	-72.50	kJ/mol	Joback Method
hf	-451.58	kJ/mol	Joback Method
hfus	19.03	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.803		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1580.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1558.00		NIST Webbook
tb	686.37	K	Joback Method
tc	938.78	K	Joback Method
tf	460.67	K	Joback Method
vc	0.757	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.71	J/molxK	686.37	Joback Method
cpg	627.81	J/molxK	728.44	Joback Method
cpg	649.33	J/molxK	770.51	Joback Method

cpg	670.71	J/mol×K	812.57	Joback Method
cpg	692.36	J/mol×K	854.64	Joback Method
cpg	714.72	J/mol×K	896.71	Joback Method
cpg	738.19	J/mol×K	938.78	Joback Method

## Sources

<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=R131501&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R131501&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<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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