

# abscisic acid, Me

<b>Inchi:</b>	InChI=1S/C15H20O4/c1-11(9-13(17)19-4)5-7-15(18)8-6-12(16)10-14(15,2)3/h5-9,18H,10
<b>InchiKey:</b>	UKAUFLFABWQUBS-GJIHDBRLSA-N
<b>Formula:</b>	C15H20O4
<b>SMILES:</b>	<chem>COC(=O)C=C(C)C=CC1(O)C=CC(=O)CC1(C)C</chem>
<b>Mol. weight [g/mol]:</b>	264.32

## Physical Properties

Property code	Value	Unit	Source
gf	-230.30	kJ/mol	Joback Method
hf	-540.77	kJ/mol	Joback Method
hfus	21.62	kJ/mol	Joback Method
hvap	77.17	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.948		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	801.61	K	Joback Method
tc	1023.64	K	Joback Method
tf	487.59	K	Joback Method
vc	0.800	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.35	J/molxK	801.61	Joback Method
cpg	656.10	J/molxK	838.62	Joback Method
cpg	672.88	J/molxK	875.62	Joback Method
cpg	689.89	J/molxK	912.63	Joback Method
cpg	707.34	J/molxK	949.63	Joback Method
cpg	725.44	J/molxK	986.64	Joback Method
cpg	744.38	J/molxK	1023.64	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=R282585&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R282585&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>rinpola:</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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