

# Guaiacyl angelate

<b>Inchi:</b>	InChI=1S/C12H14O3/c1-4-9(2)12(13)15-11-8-6-5-7-10(11)14-3/h4-8H,1-3H3/b9-4-
<b>InchiKey:</b>	MNXOFCMTJXDHDP-WTKPLQERSA-N
<b>Formula:</b>	C12H14O3
<b>SMILES:</b>	CC=C(C)C(=O)Oc1ccccc1OC
<b>Mol. weight [g/mol]:</b>	206.24

## Physical Properties

Property code	Value	Unit	Source
gf	-114.31	kJ/mol	Joback Method
hf	-335.54	kJ/mol	Joback Method
hfus	23.36	kJ/mol	Joback Method
hvap	56.85	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.567		Crippen Method
mvol	165.190	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
ripol	2219.00		NIST Webbook
tb	608.37	K	Joback Method
tc	825.53	K	Joback Method
tf	339.29	K	Joback Method
vc	0.623	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.54	J/molxK	608.37	Joback Method
cpg	412.85	J/molxK	644.56	Joback Method
cpg	426.33	J/molxK	680.76	Joback Method
cpg	439.00	J/molxK	716.95	Joback Method
cpg	450.87	J/molxK	753.14	Joback Method
cpg	461.96	J/molxK	789.34	Joback Method
cpg	472.29	J/molxK	825.53	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R639199&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R639199&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>riPOL:</b>	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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