

# GA9(w2,3), Me

<b>Inchi:</b>	InChI=1S/C20H24O4/c1-11-9-19-10-12(11)5-6-13(19)20-8-4-7-18(2,17(22)24-20)15(20)1
<b>InchiKey:</b>	VWPPKHJWYLVPPJJ-SJOHMHBKSA-N
<b>Formula:</b>	C20H24O4
<b>SMILES:</b>	<chem>C=C1CC23CC1CCC2C12CC=CC(C)(C(=O)O1)C2C3C(=O)OC</chem>
<b>Mol. weight [g/mol]:</b>	328.40

## Physical Properties

Property code	Value	Unit	Source
gf	5.59	kJ/mol	Joback Method
hf	-471.89	kJ/mol	Joback Method
hfus	27.62	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.030		Crippen Method
mvol	244.640	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	2333.00		NIST Webbook
rinpol	2333.00		NIST Webbook
tb	860.00	K	Joback Method
tc	1111.71	K	Joback Method
tf	642.43	K	Joback Method
vc	0.939	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.88	J/molxK	860.00	Joback Method
cpg	883.23	J/molxK	901.95	Joback Method
cpg	911.08	J/molxK	943.90	Joback Method
cpg	941.00	J/molxK	985.85	Joback Method
cpg	973.57	J/molxK	1027.81	Joback Method
cpg	1009.34	J/molxK	1069.76	Joback Method
cpg	1048.91	J/molxK	1111.71	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R80095&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R80095&amp;Units=SI</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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