

# Decalin, 2-methylene-5,5,8a-trimethyl-1-(2,5-dimethoxybenzyl)-4a«alpha»-

InChI: InChI=1S/C23H34O2/c1-16-8-11-21-22(2,3)12-7-13-23(21,4)19(16)15-17-14-18(24-5)9-10  
InChIKey: LULQAZFDPUGEBU-UHFFFAOYSA-N

Formula: C23H34O2

SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1Cc1cc(OC)ccc1OC

Mol. weight [g/mol]: 342.51

## Physical Properties

Property code	Value	Unit	Source
gf	125.71	kJ/mol	Joback Method
hf	-373.90	kJ/mol	Joback Method
hfus	27.22	kJ/mol	Joback Method
hvap	72.96	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	6.045		Crippen Method
mcvol	296.890	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinsol	2488.00		NIST Webbook
tb	827.98	K	Joback Method
tc	1057.31	K	Joback Method
tf	519.69	K	Joback Method
vc	1.111	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.30	J/molxK	827.98	Joback Method
cpg	993.77	J/molxK	866.20	Joback Method
cpg	1018.79	J/molxK	904.42	Joback Method
cpg	1043.60	J/molxK	942.65	Joback Method
cpg	1068.45	J/molxK	980.87	Joback Method
cpg	1093.57	J/molxK	1019.09	Joback Method
cpg	1119.20	J/molxK	1057.31	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=U195820&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U195820&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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