

# 2-Dimethylamino-8(ar)-methoxy-tetrahydro-1-acer

<b>Inchi:</b>	InChI=1S/C16H21NO2/c1-17(2)9-12-11-6-4-5-10-7-8-13(19-3)15(14(10)11)16(12)18/h7-
<b>InchiKey:</b>	QXXUCXAVKQQQEZ-UHFFFAOYSA-N
<b>Formula:</b>	C16H21NO2
<b>SMILES:</b>	COc1ccc2c3c1C(=O)C(CN(C)C)C3CCC2
<b>Mol. weight [g/mol]:</b>	259.34
<b>CAS:</b>	116296-20-9

## Physical Properties

Property code	Value	Unit	Source
gf	172.05	kJ/mol	Joback Method
hf	-228.24	kJ/mol	Joback Method
hfus	30.06	kJ/mol	Joback Method
hvap	64.00	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.489		Crippen Method
mcvol	208.240	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
tb	723.26	K	Joback Method
tc	947.48	K	Joback Method
tf	492.86	K	Joback Method
vc	0.780	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.97	J/molxK	723.26	Joback Method
cpg	640.28	J/molxK	760.63	Joback Method
cpg	657.42	J/molxK	798.00	Joback Method
cpg	673.43	J/molxK	835.37	Joback Method
cpg	688.40	J/molxK	872.74	Joback Method
cpg	702.37	J/molxK	910.11	Joback Method
cpg	715.40	J/molxK	947.48	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=C116296209&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116296209&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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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