

# 2H-1,3-Oxazine, tetrahydro-2-(4-methoxyphenyl)-

<b>Other names:</b>	2-(4'-Methoxyphenyl)perhydro-1,3-oxazine
<b>Inchi:</b>	InChI=1S/C11H15NO2/c1-13-10-5-3-9(4-6-10)11-12-7-2-8-14-11/h3-6,11-12H,2,7-8H2,1
<b>InchiKey:</b>	CATPMMKKMWYOSJ-UHFFFAOYSA-N
<b>Formula:</b>	C11H15NO2
<b>SMILES:</b>	<chem>COc1ccc(C2NCCCO2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	193.24
<b>CAS:</b>	109086-77-3

## Physical Properties

Property code	Value	Unit	Source
gf	65.56	kJ/mol	Joback Method
hf	-217.40	kJ/mol	Joback Method
hfus	28.49	kJ/mol	Joback Method
hvap	57.12	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.704		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
tb	600.21	K	Joback Method
tc	844.12	K	Joback Method
tf	413.88	K	Joback Method
vc	0.552	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.17	J/molxK	600.21	Joback Method
cpg	408.57	J/molxK	640.86	Joback Method
cpg	425.75	J/molxK	681.51	Joback Method
cpg	441.73	J/molxK	722.16	Joback Method
cpg	456.50	J/molxK	762.81	Joback Method
cpg	470.09	J/molxK	803.47	Joback Method
cpg	482.52	J/molxK	844.12	Joback Method

# Sources

<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>
<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=C109086773&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C109086773&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>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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