

# Benzoxazole, 2-methyl-

<b>Other names:</b>	2-Methylbenzoxazole USAF ek-982 2-Methylbenzoxazol
<b>Inchi:</b>	InChI=1S/C8H7NO/c1-6-9-7-4-2-3-5-8(7)10-6/h2-5H,1H3
<b>InchiKey:</b>	DQSHFKPKFISSNM-UHFFFAOYSA-N
<b>Formula:</b>	C8H7NO
<b>SMILES:</b>	Cc1nc2ccccc2o1
<b>Mol. weight [g/mol]:</b>	133.15
<b>CAS:</b>	95-21-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.25		Crippen Method
logp	2.136		Crippen Method
mcvol	100.510	ml/mol	McGowan Method
tb	451.20	K	NIST Webbook
tb	473.70	K	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.70	K	1.60	NIST Webbook

## Sources

<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=C95216&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C95216&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure

Latest version available from:

<https://www.cheméo.com/cid/26-974-2/Benzoxazole-2-methyl.pdf>

Generated by Cheméo on 2024-04-26 19:58:15.146436197 +0000 UTC m=+16450744.067013512.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.