

# Benzofuran, 2-methyl-

<b>Other names:</b>	2-METHYLBENZOFURAN 2-METHYLCUMARONE 2-Methylbenzo[b]furan
<b>Inchi:</b>	InChI=1S/C9H8O/c1-7-6-8-4-2-3-5-9(8)10-7/h2-6H,1H3
<b>InchiKey:</b>	GBGPVUAOTCNZPT-UHFFFAOYSA-N
<b>Formula:</b>	C9H8O
<b>SMILES:</b>	Cc1cc2ccccc2o1
<b>Mol. weight [g/mol]:</b>	132.16
<b>CAS:</b>	4265-25-2

## Physical Properties

Property code	Value	Unit	Source
affp	859.60	kJ/mol	NIST Webbook
basg	827.20	kJ/mol	NIST Webbook
log10ws	-7.49		Crippen Method
logp	2.741		Crippen Method
mcvol	104.620	ml/mol	McGowan Method
rinpol	184.50		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	180.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1563.00		NIST Webbook
tb	470.70	K	NIST Webbook

## Correlations

Information	Value
Property code	pvap

Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46238e+01
Coeff. B	-4.06751e+03
Coeff. C	-6.36230e+01
Temperature range (K), min.	347.35
Temperature range (K), max.	500.41

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>KDB:</b>	<a href="https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1040">https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1040</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=C4265252&amp;Units=S1">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4265252&amp;Units=S1</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<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>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

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