Benzofuran, 2-methyl-

Other names:	2-METHYLBENZOFURAN
	2-METHYLCUMARONE
	2-Methylbenzo[b]furan
Inchi:	InChI=1S/C9H8O/c1-7-6-8-4-2-3-5-9(8)10-7/h2-6H,1H3
InchiKey:	GBGPVUAOTCNZPT-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	Cc1cc2ccccc2o1
Mol. weight [g/mol]:	132.16
CAS:	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	1109.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	180.00		NIST Webbook
rinpol	184.50		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1123.00		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(Pvp) = 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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4265252&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1040
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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