1H-Pyrrole, 2-methyl-

Other names:	2-Methylpyrrole
	2-methyl-1H-pyrrole
	Pyrrole, 2-methyl-
	«alpha»-Methylpyrrole
	Â«alphaÂ»-Methylpyrrole
Inchi:	InChI=1S/C5H7N/c1-5-3-2-4-6-5/h2-4,6H,1H3
InchiKey:	TVCXVUHHCUYLGX-UHFFFAOYSA-N
Formula:	C5H7N
SMILES:	Cc1ccc[nH]1
Mol. weight [g/mol]:	81.12
CAS:	636-41-9

Physical Properties

Property code	Value	Unit	Source
ie	7.78 ± 0.01	eV	NIST Webbook
ie	8.01 ± 0.05	eV	NIST Webbook
log10ws	-1.17		Crippen Method
logp	0.841		Crippen Method
mcvol	71.830	ml/mol	McGowan Method
rinpol	812.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	853.00		NIST Webbook
ripol	1551.00		NIST Webbook

ripol	1575.00		NIST Webbook
ripol	1590.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1549.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1562.00		NIST Webbook
tb	421.00 ± 2.00	K	NIST Webbook
tb	421.15 ± 2.00	K	NIST Webbook
tb	420.65 ± 0.50	K	NIST Webbook
tb	421.15 ± 2.00	K	NIST Webbook
tf	237.55 ± 0.30	K	NIST Webbook
tf	237.55 ± 0.40	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49887e+01
Coeff. B	-3.76320e+03
Coeff. C	-5.81180e+01
Temperature range (K), min.	314.10
Temperature range (K), max.	446.99

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C636419&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

Legend

ie:	Ionization energy
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
tf:	Normal melting (fusion) point