1H-Pyrrole, 3-methyl-

Other names:	3-Methylpyrrole
	3-methyl-1H-pyrrole
	Pyrrole, 3-methyl-
Inchi:	InChI=1S/C5H7N/c1-5-2-3-6-4-5/h2-4,6H,1H3
InchiKey:	FEKWWZCCJDUWLY-UHFFFAOYSA-N
Formula:	C5H7N
SMILES:	Cc1cc[nH]c1
Mol. weight [g/mol]:	81.12
CAS:	616-43-3

Physical Properties

Property code	Value	Unit	Source
ie	7.90 ± 0.02	eV	NIST Webbook
log10ws	-1.17		Crippen Method
logp	0.841		Crippen Method
mcvol	71.830	ml/mol	McGowan Method
rinpol	860.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	862.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1569.00		NIST Webbook
tb	416.00 ± 2.00	K	NIST Webbook
tb	416.00 ± 1.50	K	NIST Webbook
tf	224.75 ± 0.30	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50098e+01
Coeff. B	-3.73249e+03
Coeff. C	-5.68120e+01
Temperature range (K), min.	310.34
Temperature range (K), max.	441.67

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C616433&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:
https://www.chemeo.com/cid/17-577-3/1H-Pyrrole-3-methyl.pdf
Generated by Cheméo on 2024-10-12 04:19:28.522164124 +0000 UTC m=+3287631.159133372.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.