

1H-Pyrrole, 1-butyl-

Other names:	1-Butyl-1H-pyrrole 1-Butylpyrrole 1-n-Butylpyrrole N-Butylpyrrole Pyrrole, 1-butyl- Pyrrole, 1-n-butyl-
Inchi:	InChI=1S/C8H13N/c1-2-3-6-9-7-4-5-8-9/h4-5,7-8H,2-3,6H2,1H3
InchiKey:	IIYSNNBEZBAQCQ-UHFFFAOYSA-N
Formula:	C8H13N
SMILES:	CCCCn1cccc1
Mol. weight [g/mol]:	123.20
CAS:	589-33-3

Physical Properties

Property code	Value	Unit	Source
ie	7.87 ± 0.02	eV	NIST Webbook
log10ws	-2.57		Crippen Method
logp	2.288		Crippen Method
mcvol	114.100	ml/mol	McGowan Method
rinpol	986.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	986.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1342.00		NIST Webbook
tf	207.05 ± 0.30	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45685e+01
Coeff. B	-3.82420e+03

Coeff. C	-6.44850e+01
Temperature range (K), min.	332.27
Temperature range (K), max.	477.60

Sources

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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C589333&Units=SI

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
tf:	Normal melting (fusion) point

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