

1-Butylpyrrolidine

Other names:	Pyrrolidine, 1-butyl- n-Butylpyrrolidine N-bButyl-tetrahydropyrrole N-butyl-Tetrahydropyrrole
Inchi:	InChI=1S/C8H17N/c1-2-3-6-9-7-4-5-8-9/h2-8H2,1H3
InchiKey:	JSHASCFKOSDFHY-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CCCCN1CCCC1
Mol. weight [g/mol]:	127.23
CAS:	767-10-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	1.882		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
rinpol	954.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	939.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1082.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.20	K	101.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C767102&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure

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