

2-Pyrrolidinone, 1-butyl-

Other names:	1-Butyl-2-pyrrolidione 1-butyl-2-pyrrolidinone 1-butyl-2-pyrrolidone 1-butylpyrrolidin-2-one N-Butylpyrrolidinone N-Butylpyrrolidone N-butyl-2-pyrrolidinone N-butyl-2-pyrrolidone N-butylbutyrolactam N-n-Butyl-2-pyrrolidone
Inchi:	InChI=1S/C8H15NO/c1-2-3-6-9-7-4-5-8(9)10/h2-7H2,1H3
InchiKey:	BNXZHVUCNYMNOS-UHFFFAOYSA-N
Formula:	C8H15NO
SMILES:	CCCCN1CCCC1=O
Mol. weight [g/mol]:	141.21
CAS:	3470-98-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.41		Crippen Method
logp	1.409		Crippen Method
mcvol	124.270	ml/mol	McGowan Method
ripol	2236.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3470982&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Phase behaviour for the (CO₂ + 1-butyl-2-pyrrolidone) and (CO₂ + N-butyl-2-pyrrolidone) systems at temperatures from (313.2 to 393.2) K and pressures up to 28 MPa: <https://www.doi.org/10.1016/j.jct.2018.10.002>

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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