

1-(3-Aminopropyl)-2-pyrrolidone

Other names:	2-Pyrrolidinone, 1-(3-aminopropyl)- N-(3-Aminopropyl)-2-pyrrolidinone 1-(3-Aminopropyl)-2-pyrrolidinone N-(3-aminopropyl)pyrrolidin-2-one
Inchi:	InChI=1S/C7H14N2O/c8-4-2-6-9-5-1-3-7(9)10/h1-6,8H2
InchiKey:	HJORCZCMNWLHMB-UHFFFAOYSA-N
Formula:	C7H14N2O
SMILES:	NCCCN1CCCC1=O
Mol. weight [g/mol]:	142.20
CAS:	7663-77-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.43		Crippen Method
logp	-0.042		Crippen Method
mcvol	120.160	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.70	K	0.10	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7663776&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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