

1-Pyrrolidinebutyronitrile

Other names:	4-Pyrrolidinylbutanenitrile 4-Pyrrolidinobutyronitrile 1-Pyrrolidinebutanenitrile 4-(1-Pyrrolidine)butyronitrile 4-pyrrolidin-1-ylbutyronitrile
Inchi:	InChI=1S/C8H14N2/c9-5-1-2-6-10-7-3-4-8-10/h1-4,6-8H2
InchiKey:	OSDDDHPYSNZBPF-UHFFFAOYSA-N
Formula:	C8H14N2
SMILES:	N#CCCCN1CCCC1
Mol. weight [g/mol]:	138.21
CAS:	35543-25-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	1.386		Crippen Method
mcvol	124.080	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35543250&Units=SI
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

Legend

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

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