N-(2-Cyanoethyl)-pyrrole

Other names:	1H-Pyrrole-1-propanenitrile
	Pyrrole-1-propionitrile
	1-(2-Cyanoethyl)pyrrole
	3-Pyrrolidinopropionitrile
	3-(pyrrol-1-yl)propiononitrile
Inchi:	InChI=1S/C7H8N2/c8-4-3-7-9-5-1-2-6-9/h1-2,5-6H,3,7H2
InchiKey:	IYOLJLGYJMJLSU-UHFFFAOYSA-N
Formula:	C7H8N2
SMILES:	N#CCCn1cccc1
Mol. weight [g/mol]:	120.15
CAS:	43036-06-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	1.402		Crippen Method
mcvol	101.390	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.70	K	1.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C43036062&Units=SI
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

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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