(S)-(+)-1-(2-Pyrrolidinylmethyl)-pyrrolidine

Inchi: InChI=1S/C9H18N2/c1-2-7-11(6-1)8-9-4-3-5-10-9/h9-10H,1-8H2/t9-/m0/s1
InchiKey: YLBWRMSQRFEIEB-VIFPVBQESA-N
Formula: C9H18N2
SMILES: C1CNC(CN2CCCC2)C1
Mol. weight [g/mol]: 154.25
CAS: 51207-66-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	0.834		Crippen Method
mcvol	135.910	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.20	K	0.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51207660&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
tbrp:	Boiling point at reduced pressure

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