(S)-(-)-1-Amino-2-(methoxymethyl)-pyrrolidine

Inchi: InChI=1S/C6H14N2O/c1-9-5-6-3-2-4-8(6)7/h6H,2-5,7H2,1H3/t6-/m1/s1
InchiKey: BWSIKGOGLDNQBZ-ZCFIWIBFSA-N
Formula: C6H14N2O
SMILES: COCC1CCCN1N
Mol. weight [g/mol]: 130.19
CAS: 59983-39-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.42		Crippen Method
logp	-0.029		Crippen Method
mcvol	110.370	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	315.20	K	0.30	NIST Webbook

Sources

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=C59983390&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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