(S)-(-)-2-(Methoxymethyl)-1-pyrrolidinecarboxalde

Inchi: InChI=1S/C7H13NO2/c1-10-5-7-3-2-4-8(7)6-9/h6-7H,2-5H2,1H3/t7-/m1/s1
InchiKey: JNIOQRWRORXADR-SSDOTTSWSA-N
Formula: C7H13NO2
SMILES: COCC1CCCN1C=O
Mol. weight [g/mol]: 143.18
CAS: 63126-45-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.19		Crippen Method
logp	0.254		Crippen Method
mcvol	116.050	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.20	K	0.04	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=C63126454&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