

# (S)-(-)-2-(Methoxymethyl)-1-pyrrolidinecarboxaldehyde

**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](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/ci9903071>

## 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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