4-Pyrrolidinobenzaldehyde

Other names:	Benzaldehyde, 4-(1-pyrrolidinyl)- 4-Pyrrolidinnobenzaldehyde 4-(1-pyrrolidinyl)benzaldehyde
Inchi:	InChI=1S/C11H13NO/c13-9-10-3-5-11(6-4-10)12-7-1-2-8-12/h3-6,9H,1-2,7-8H2
InchiKey:	DATXHLPRESKQJK-UHFFFAOYSA-N
Formula:	C11H13NO
SMILES:	O=Cc1ccc(N2CCCC2)cc1
Mol. weight [g/mol]:	175.23
CAS:	51980-54-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	2.099		Crippen Method
mcvol	142.780	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51980542&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume