N-Formyltryptamine

Inchi: InChI=1S/C11H12N2O/c14-8-12-6-5-9-7-13-11-4-2-1-3-10(9)11/h1-4,7-8,13H,5-6H2,(H,1
InchiKey: JQWVVJKFXINLNV-UHFFFAOYSA-N
Formula: C11H12N2O
SMILES: OC=NCCc1c[nH]c2ccccc12
Mol. weight [g/mol]: 188.23
CAS: 6502-82-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.815		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
rinpol	2216.30		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6502825&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
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.