

Janfestine

Inchi: InChI=1S/C9H15NO3/c1-13-9(12)6-2-4-10-5-3-7(11)8(6)10/h6-8,11H,2-5H2,1H3/t6-,7+,8-
InchiKey: RXRCQXLXRSNQCP-CSMHCCOUSA-N
Formula: C9H15NO3
SMILES: COC(=O)C1CCN2CCC(O)C12
Mol. weight [g/mol]: 185.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.06		Crippen Method
logp	-0.385		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
rinpola	1485.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R335278&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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/15-909-6/Janfestine.pdf>

Generated by Cheméo on 2024-04-27 15:02:20.2260006 +0000 UTC m=+16519389.146577922.

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