

5,6-Dehydro-«alpha»-isolupanine

Inchi: InChI=1S/C15H22N2O/c18-15-6-3-5-14-11-8-12(10-17(14)15)13-4-1-2-7-16(13)9-11/h3,6-14,17-18
InchiKey: YDYCLZUDFBNNQE-XUXIUFHCSA-N
Formula: C15H22N2O
SMILES: O=C1C=CCC2C3CC(CN12)C1CCCCN1C3
Mol. weight [g/mol]: 246.35

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.19 | | Crippen Method |
| logp | 1.648 | | Crippen Method |
| mcvol | 196.000 | ml/mol | McGowan Method |
| rinpol | 2052.00 | | NIST Webbook |
| rinpol | 2075.00 | | NIST Webbook |
| rinpol | 2070.00 | | NIST Webbook |
| rinpol | 2052.00 | | NIST Webbook |
| rinpol | 2070.00 | | 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=R264067&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/30-564-2/5-6-Dehydro-alpha-isolupanine.pdf>

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