# Rinderine

**Inchi:** InChI=1S/C15H27NO5/c1-9(2)15(20,10(3)17)14(19)21-8-11-4-6-16-7-5-12(18)13(11)16/h
**InchiKey:** NMPPLGMVCCNRTJ-UHFFFAOYSA-N
**Formula:** C15H27NO5
**SMILES:** CC(C)C(O)(C(=O)OCC1CCN2CCC(O)C12)C(C)O
**Mol. weight [g/mol]:** 301.38
**CAS:** 6029-84-1

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -1.08 | | Crippen Method |
| logp | -0.247 | | Crippen Method |
| mcvol | 235.520 | ml/mol | McGowan Method |
| rinpol | 2155.00 | | NIST Webbook |
| rinpol | 2155.00 | | NIST Webbook |
| rinpol | 2153.00 | | NIST Webbook |
| rinpol | 2150.00 | | NIST Webbook |
| rinpol | 2152.00 | | NIST Webbook |
| rinpol | 2152.00 | | NIST Webbook |
| rinpol | 2152.00 | | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C6029841&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 |

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https://www.chemeo.com/cid/57-868-6/Rinderine.pdf

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