

Echimidine

Inchi: InChI=1S/C20H31NO7/c1-6-12(2)17(23)28-15-8-10-21-9-7-14(16(15)21)11-27-18(24)20
InchiKey: HRSGCYGUWHGOPY-IMYHSKLDSA-N
Formula: C20H31NO7
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)O)C(C)(C)O)C12
Mol. weight [g/mol]: 397.46
CAS: 520-68-3

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.34 | | Crippen Method |
| logp | 0.305 | | Crippen Method |
| mcvol | 304.810 | ml/mol | McGowan Method |
| rinpola | 2560.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C520683&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

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<https://www.chemeo.com/cid/30-886-5/Echimidine.pdf>

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