

Galanthan-1-ol, 3,12-didehydro-9,10-[methylenebis(oxy)]-, (1«alpha»)-

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|----------------------|---|
| Other names: | Lycoran-1 «alpha»-ol, 3,3a-didehydro-Caranin Caranine Galanthan-1-ol, 3,4-didehydro-11,12-[methylenebis(oxy)]-, (1 «alpha»)- (1R,3a1S,12bS)-2,3a1,4,5,7,12b-Hexahydro-1H-[1,3]dioxolo[4,5- <i>j</i>]pyrrolo[3,2,1- <i>de</i>]phena |
| Inchi: | InChI=1S/C16H17NO3/c18-12-2-1-9-3-4-17-7-10-5-13-14(20-8-19-13)6-11(10)15(12)16(|
| InchiKey: | XKYSLILSDJBMCU-UHFFFAOYSA-N |
| Formula: | C16H17NO3 |
| SMILES: | OC1CC=C2CCN3Cc4cc5c(cc4C1C23)OCO5 |
| Mol. weight [g/mol]: | 271.31 |
| CAS: | 477-12-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.43 | | Crippen Method |
| logp | 1.778 | | Crippen Method |
| mcvol | 192.390 | ml/mol | McGowan Method |
| rinpol | 2524.10 | | NIST Webbook |
| rinpol | 2524.10 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C477123&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

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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