

10,17-Dioxo-«beta»-sparteine

Inchi: InChI=1S/C15H22N2O2/c18-14-10-9-16-7-3-1-6-12(16)13(14)15(19)17-8-4-2-5-11(10)17
InchiKey: ALRKCTGHXZGXNU-UHFFFAOYSA-N
Formula: C15H22N2O2
SMILES: O=C1C2CN3CCCCC3C1C(=O)N1CCCCC21
Mol. weight [g/mol]: 262.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Crippen Method
logp	1.051		Crippen Method
mcvol	201.870	ml/mol	McGowan Method
rinpol	2346.00		NIST Webbook
rinpol	2340.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R263782&Units=SI>

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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