

Homobaldrinal

Inchi: InChI=1S/C15H16O4/c1-10(2)5-15(17)19-8-12-7-18-9-14-11(6-16)3-4-13(12)14/h3-4,6-7
InchiKey: LTVSLKWNAZKBEX-UHFFFAOYSA-N
Formula: C15H16O4
SMILES: CC(C)CC(=O)OCc1cocc2c(C=O)ccc1-2
Mol. weight [g/mol]: 260.29
CAS: 67910-07-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.06		Crippen Method
logp	3.286		Crippen Method
mcvol	198.170	ml/mol	McGowan Method
rinpol	2154.40		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=C67910070&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

Latest version available from:

<https://www.chemeo.com/cid/84-953-1/Homobaldrinal.pdf>

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