

Benzoic acid, 4-[1-hydroxy-2-(2-oxopyrrolidino)hexyl]-, ethyl ester

Other names: R,S-4'-methyl-«alpha»-pyrrolidinohexanophenone-M (oxo-carboxy-dihydro-), ethylated
Inchi: InChI=1S/C19H27NO4/c1-3-5-7-16(20-13-6-8-17(20)21)18(22)14-9-11-15(12-10-14)19(20)2
InchiKey: FCBAEBYCZGRVFB-UHFFFAOYSA-N
Formula: C19H27NO4
SMILES: CCCCC(C(O)c1ccc(C(=O)OCC)cc1)N1CCCC1=O
Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	3.078		Crippen Method
mcvol	268.810	ml/mol	McGowan Method
rinpol	2620.00		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=U314305&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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