1-Methyl-4-piperidyl cyclohexylphenylglycolate

Inchi: InChI=1S/C20H29NO3/c1-21-14-12-18(13-15-21)24-19(22)20(23,16-8-4-2-5-9-16)17-10-

InchiKey: QZPMHVOJMAXMND-UHFFFAOYSA-N

Formula: C20H29NO3

SMILES: CN1CCC(OC(=O)C(O)(c2ccccc2)C2CCCCC2)CC1

Mol. weight [g/mol]: 331.45

CAS: 33445-17-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	3.092		Crippen Method
mcvol	270.470	ml/mol	McGowan Method
rinpol	2408.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33445179&Units=SI

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

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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