4-Ethylbenzoic acid, morpholide

Inchi: InChI=1S/C13H17NO2/c1-2-11-3-5-12(6-4-11)13(15)14-7-9-16-10-8-14/h3-6H,2,7-10H2,
InchiKey: JYYGRJIDXBRVHD-UHFFFAOYSA-N
Formula: C13H17NO2
SMILES: CCc1ccc(C(=O)N2CCOCC2)cc1
Mol. weight [g/mol]: 219.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.721		Crippen Method
mcvol	176.830	ml/mol	McGowan Method
rinpol	1874.00		NIST Webbook
rinpol	1874.00		NIST Webbook

Sources

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=U307011&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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