L-Proline, N-(3-methoxybenzoyl)-, isobutyl ester

Inchi: InChI=1S/C17H23NO4/c1-12(2)11-22-17(20)15-8-5-9-18(15)16(19)13-6-4-7-14(10-13)21
InchiKey: GQCVPDVHIIWZQU-UHFFFAOYSA-N
Formula: C17H23NO4
SMILES: COc1cccc(C(=O)N2CCCC2C(=O)OCC(C)C)c1
Mol. weight [g/mol]: 305.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	2.499		Crippen Method
mcvol	240.630	ml/mol	McGowan Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		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=U346168&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.