5-(benzoyl)-2,3-dihydro-1H-pyrrolizine-1-carboxyli acid

Inchi: InChI=1S/C15H13NO3/c17-14(10-4-2-1-3-5-10)13-7-6-12-11(15(18)19)8-9-16(12)13/h1-
InchiKey: OZWKMVRBQXNZKK-UHFFFAOYSA-N
Formula: C15H13NO3
SMILES: O=C(c1ccccc1)c1ccc2n1CCC2C(=O)O
Mol. weight [g/mol]: 255.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Aqueous Solubility Prediction Method
logp	2.291		Crippen Method
mcvol	187.120	ml/mol	McGowan Method
tf	433.65	K	Aqueous Solubility Prediction Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
tf: Normal melting (fusion) point

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