4-Nitrobenzoic acid, morpholide

Inchi: InChI=1S/C11H12N2O4/c14-11(12-5-7-17-8-6-12)9-1-3-10(4-2-9)13(15)16/h1-4H,5-8H2
InchiKey: VGGZQWDRWOXJTA-UHFFFAOYSA-N
Formula: C11H12N2O4
SMILES: O=C(c1ccc([N+](=O)[O-])cc1)N1CCOCC1
Mol. weight [g/mol]: 236.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	1.067		Crippen Method
mcvol	166.070	ml/mol	McGowan Method
rinpol	2079.00		NIST Webbook
rinpol	2079.00		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=U307348&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.