4-Azidobenzoic acid

Other names:	p-Azidobenzoic acid
	Benzoic acid, 4-azido-
Inchi:	InChI=1S/C7H5N3O2/c8-10-9-6-3-1-5(2-4-6)7(11)12/h1-4H,(H,11,12)
InchiKey:	PQXPAFTXDVNANI-UHFFFAOYSA-N
Formula:	C7H5N3O2
SMILES:	[N-]=[N+]=Nc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	163.13
CAS:	6427-66-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.19		Crippen Method
logp	2.327		Crippen Method
mcvol	114.510	ml/mol	McGowan Method

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=C6427663&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

Latest version available from:
https://www.chemeo.com/cid/39-070-1/4-Azidobenzoic-acid.pdf
Generated by Cheméo on 2025-12-05 17:17:29.649108498 +0000 UTC m=+4703247.179149152.

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