Picolinamide, 5-nitro-

Inchi: InChI=1S/C6H5N3O3/c7-6(10)5-2-1-4(3-8-5)9(11)12/h1-3H,(H2,7,10)
InchiKey: JGLGOTZFQGEALJ-UHFFFAOYSA-N
Formula: C6H5N3O3
SMILES: NC(=O)c1ccc([N+](=O)[O-])cn1
Mol. weight [g/mol]: 167.12
CAS: 59290-34-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	0.089		Crippen Method
mcvol	110.590	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59290345&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:
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