2-Furoylacetonitrile

Inchi: InChI=1S/C7H5NO2/c8-4-3-6(9)7-2-1-5-10-7/h1-2,5H,3H2
InchiKey: RZNSHBXVTAHWPP-UHFFFAOYSA-N
Formula: C7H5NO2
SMILES: N#CCC(=O)c1ccco1
Mol. weight [g/mol]: 135.12
CAS: 31909-58-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.15		Crippen Method
logp	1.376		Crippen Method
mcvol	98.850	ml/mol	McGowan Method

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=C31909587&Units=SI

Legend

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