2-Pyridinesulfonylacetonitrile

Inchi: InChI=1S/C7H6N2O2S/c8-4-6-12(10,11)7-3-1-2-5-9-7/h1-3,5H,6H2
InchiKey: SAKACXZDAJXBCI-UHFFFAOYSA-N
Formula: C7H6N2O2S
SMILES: N#CCS(=O)(=O)c1ccccn1
Mol. weight [g/mol]: 182.20
CAS: 170449-34-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.22		Crippen Method
logp	0.379		Crippen Method
mcvol	125.180	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C170449340&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