2-Thiopheneacetic acid, morpholide

Inchi: InChI=1S/C10H13NO2S/c12-10(8-9-2-1-7-14-9)11-3-5-13-6-4-11/h1-2,7H,3-6,8H2
InchiKey: YQYAJHBIKRXEGG-UHFFFAOYSA-N
Formula: C10H13NO2S
SMILES: O=C(Cc1cccs1)N1CCOCC1
Mol. weight [g/mol]: 211.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	1.149		Crippen Method
mcvol	155.210	ml/mol	McGowan Method
rinpol	1770.00		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=U306899&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