2-Thiopheneacetamide, N-(2-fluorophenyl)-

Inchi: InChI=1S/C12H10FNOS/c13-10-5-1-2-6-11(10)14-12(15)8-9-4-3-7-16-9/h1-7H,8H2,(H,14
InchiKey: XNLZAHXIARXVLQ-UHFFFAOYSA-N
Formula: C12H10FNOS
SMILES: O=C(Cc1cccs1)Nc1ccccc1F
Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	3.068		Crippen Method
mcvol	166.390	ml/mol	McGowan Method
rinpol	1883.00		NIST Webbook
rinpol	1883.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308134&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
rinpol: Non-polar retention indices

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