

Acetamide, N-(3-nitrophenyl)-2-(2-thienyl)-

Inchi: InChI=1S/C12H10N2O3S/c15-12(8-11-5-2-6-18-11)13-9-3-1-4-10(7-9)14(16)17/h1-7H,8H
InchiKey: OZYGTPZTXULJW-UHFFFAOYSA-N
Formula: C12H10N2O3S
SMILES: O=C(Cc1cccs1)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 262.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Crippen Method
logp	2.837		Crippen Method
mcvol	182.040	ml/mol	McGowan Method
rinsol	2410.00		NIST Webbook
rinsol	2410.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U306907&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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