Thiophene-2-carboxamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C11H8N2O3S/c14-11(10-5-2-6-17-10)12-8-3-1-4-9(7-8)13(15)16/h1-7H,(H,12,
InchiKey: VFDHCXRHENGDQA-UHFFFAOYSA-N
Formula: C11H8N2O3S
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)c1cccs1
Mol. weight [g/mol]: 248.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	2.909		Crippen Method
mcvol	167.950	ml/mol	McGowan Method
rinpol	2435.00		NIST Webbook
rinpol	2435.00		NIST Webbook

Sources

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=U307074&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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