2-Furancarboxamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C11H8N2O4/c14-11(10-5-2-6-17-10)12-8-3-1-4-9(7-8)13(15)16/h1-7H,(H,12,14
InchiKey: VOVIUHCZEVLDNA-UHFFFAOYSA-N
Formula: C11H8N2O4
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)c1ccco1
Mol. weight [g/mol]: 232.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.83		Crippen Method
logp	2.440		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
rinpol	2164.00		NIST Webbook
rinpol	2164.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307041&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.