

2-Thiophenecarboxamide, N-butyl-N-(2-thiophenecarbonyl)-

Inchi: InChI=1S/C14H15NO2S2/c1-2-3-8-15(13(16)11-6-4-9-18-11)14(17)12-7-5-10-19-12/h4-7
InchiKey: SICQAUDIIZSPFZ-UHFFFAOYSA-N
Formula: C14H15NO2S2
SMILES: CCCCNC(=O)c1cccs1)C(=O)c1cccs1
Mol. weight [g/mol]: 293.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.892		Crippen Method
mcvol	215.020	ml/mol	McGowan Method
rinpola	2267.00		NIST Webbook
rinpola	2267.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407039&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
rinpola: Non-polar retention indices

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