

Thiophene-2-carboxamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C13H13NO3S/c1-16-9-5-6-11(17-2)10(8-9)14-13(15)12-4-3-7-18-12/h3-8H,1-2
InchiKey: KXAQMPKVFHGX-UHFFFAOYSA-N
Formula: C13H13NO3S
SMILES: COc1ccc(OC)c(NC(=O)c2cccs2)c1
Mol. weight [g/mol]: 263.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.44		Crippen Method
logp	3.018		Crippen Method
mcvol	190.450	ml/mol	McGowan Method
rinsol	2324.00		NIST Webbook
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Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307073&Units=SI>

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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