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: KXAQMPKVFWFHGX-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
rinpol	2324.00		NIST Webbook
rinpol	2324.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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