3,4-Dimethylthiophene-2,5-dicarbonitrile

Inchi: InChI=1S/C8H6N2S/c1-5-6(2)8(4-10)11-7(5)3-9/h1-2H3
InchiKey: KJJOQVQJRGSFGU-UHFFFAOYSA-N
Formula: C8H6N2S
SMILES: Cc1c(C#N)sc(C#N)c1C
Mol. weight [g/mol]: 162.21
CAS: 155632-41-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	2.108		Crippen Method
mcvol	123.230	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C155632410&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

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