

Thiophene-2-carboxamide, N-ethyl-N-methyl-

Inchi: InChI=1S/C8H11NOS/c1-3-9(2)8(10)7-5-4-6-11-7/h4-6H,3H2,1-2H3
InchiKey: XUNYTSUFGLFFSF-UHFFFAOYSA-N
Formula: C8H11NOS
SMILES: CCN(C)C(=O)c1cccs1
Mol. weight [g/mol]: 169.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	1.840		Crippen Method
mcvol	132.020	ml/mol	McGowan Method
rinsol	1720.00		NIST Webbook
rinsol	1720.00		NIST Webbook

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=U415301&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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