

Thiophene-2-carboxamide, N-ethyl-N-3-methylbutyl-

Inchi: InChI=1S/C12H19NOS/c1-4-13(8-7-10(2)3)12(14)11-6-5-9-15-11/h5-6,9-10H,4,7-8H2,1-3
InchiKey: FTRVBJHIPRQQHX-UHFFFAOYSA-N
Formula: C12H19NOS
SMILES: CCN(CCC(C)C)C(=O)c1cccs1
Mol. weight [g/mol]: 225.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	3.256		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
rinpola	2001.00		NIST Webbook
rinpola	2001.00		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=U415306&Units=SI>

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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