# Acetamide, 2-(2-thiophenyl)-N-ethyl-N-3-methylbutyl-

**Inchi:** InChI=1S/C13H21NOS/c1-4-14(8-7-11(2)3)13(15)10-12-6-5-9-16-12/h5-6,9,11H,4,7-8,10

**InchiKey:** YYZUTWTXCYUHMU-UHFFFAOYSA-N

**Formula:** C13H21NOS

**SMILES:** CCN(CCC(C)C)C(=O)Cc1cccs1

**Mol. weight [g/mol]:** 239.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.07 | | Crippen Method |
| logp | 3.185 | | Crippen Method |
| mcvol | 202.470 | ml/mol | McGowan Method |
| rinpol | 2051.00 | | NIST Webbook |
| rinpol | 2051.00 | | NIST Webbook |

## Sources

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

**Crippen Method:** https://www.chemeo.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=U415410&Units=SI

## 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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