

1,2,5-Thiadiazole-3-carboxamide, 4-(3-ethylureido)-

Inchi: InChI=1S/C6H9N5O2S/c1-2-8-6(13)9-5-3(4(7)12)10-14-11-5/h2H2,1H3,(H2,7,12)(H2,8,9)
InchiKey: XUBDIUNIULKZHE-UHFFFAOYSA-N
Formula: C6H9N5O2S
SMILES: CCNC(=O)Nc1nsnc1C(N)=O
Mol. weight [g/mol]: 215.23
CAS: 89465-63-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	-0.222		Crippen Method
mcvol	145.330	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C89465634&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/62-063-3/1-2-5-Thiadiazole-3-carboxamide-4-3-ethylureido.pdf>

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