

Thiophene-2-carboxamide, N-tetrahydrofurfuryl-

Inchi: InChI=1S/C10H13NO2S/c12-10(9-4-2-6-14-9)11-7-8-3-1-5-13-8/h2,4,6,8H,1,3,5,7H2,(H,1,2,3,4,5,6,7,8,9,10,11,12,13,14)
InchiKey: ZVEOKBMFOXDDJU-UHFFFAOYSA-N
Formula: C10H13NO2S
SMILES: O=C(NCC1CCCO1)c1cccs1
Mol. weight [g/mol]: 211.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	1.657		Crippen Method
mcvol	155.210	ml/mol	McGowan Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307067&Units=SI>
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>

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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