

2-Thiophenecarboxamide, N-butyl-

Inchi: InChI=1S/C9H13NOS/c1-2-3-6-10-9(11)8-5-4-7-12-8/h4-5,7H,2-3,6H2,1H3,(H,10,11)
InchiKey: LEVLYSPVPFOBLP-UHFFFAOYSA-N
Formula: C9H13NOS
SMILES: CCCCNC(=O)c1cccs1
Mol. weight [g/mol]: 183.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	2.278		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
rinpole	1677.00		NIST Webbook
rinpole	1677.00		NIST Webbook

Sources

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=U407023&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/97-113-9/2-Thiophenecarboxamide-N-butyl.pdf>

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