

2-Thiophenecarboxamide, N-(3-methylbutyl)-

Inchi:	InChI=1S/C10H15NOS/c1-8(2)5-6-11-10(12)9-4-3-7-13-9/h3-4,7-8H,5-6H2,1-2H3,(H,11,
InchiKey:	VNFMHXIHXJIFRW-UHFFFAOYSA-N
Formula:	C10H15NOS
SMILES:	CC(C)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	197.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	2.524		Crippen Method
mcvol	160.200	ml/mol	McGowan Method
rinsol	1743.00		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=U407024&Units=SI

Legend

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

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