2-Thiopheneacetamide, N-isobutyl-

Inchi: InChI=1S/C10H15NOS/c1-8(2)7-11-10(12)6-9-4-3-5-13-9/h3-5,8H,6-7H2,1-2H3,(H,11,12
InchiKey: FUDQFNQABWOMIS-UHFFFAOYSA-N
Formula: C10H15NOS
SMILES: CC(C)CN=C(O)Cc1cccs1
Mol. weight [g/mol]: 197.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.45		Crippen Method
logp	2.903		Crippen Method
mcvol	160.200	ml/mol	McGowan Method
rinpol	1664.00		NIST Webbook
rinpol	1664.00		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=U407005&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.