2-formyl-N-isobutylpyrrole

Inchi: InChI=1S/C9H13NO/c1-8(2)6-10-5-3-4-9(10)7-11/h3-5,7-8H,6H2,1-2H3
InchiKey: VBXJHWIPAREKFL-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: CC(C)Cn1cccc1C=O
Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.957		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
ripol	1683.00		NIST Webbook
ripol	1683.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R314786&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
ripol: Polar retention indices

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