

2-formyl-5-hydroxymethyl-N-isobutylpyrrole

Inchi: InChI=1S/C10H15NO2/c1-8(2)5-11-9(6-12)3-4-10(11)7-13/h3-4,6,8,13H,5,7H2,1-2H3
InchiKey: KRUIYHHWGBWCLH-UHFFFAOYSA-N
Formula: C10H15NO2
SMILES: CC(C)Cn1c(C=O)ccc1CO
Mol. weight [g/mol]: 181.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.71		Crippen Method
logp	1.449		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
ripol	2243.00		NIST Webbook
ripol	2243.00		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=R314751&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
ripol: Polar retention indices

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<https://www.chemeo.com/cid/90-953-4/2-formyl-5-hydroxymethyl-N-isobutylpyrrole.pdf>

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