1-(3-Methylbutyl)-pyrrol-2-carboxaldehyde

Inchi: InChI=1S/C10H15NO/c1-9(2)5-7-11-6-3-4-10(11)8-12/h3-4,6,8-9H,5,7H2,1-2H3
InchiKey: JVGRNRKMDAVBIH-UHFFFAOYSA-N
Formula: C10H15NO
SMILES: CC(C)CCn1cccc1C=O
Mol. weight [g/mol]: 165.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	2.347		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
ripol	1812.00		NIST Webbook
ripol	1821.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R547585&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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