2-formyl-5-methyl-N-isobutylpyrrole

Other names: 5-methyl-1-(2-methylpropyl)-1H-pyrrole-2-carboxaldehyde
Inchi: InChI=1S/C10H15NO/c1-8(2)6-11-9(3)4-5-10(11)7-12/h4-5,7-8H,6H2,1-3H3
InchiKey: YEIYSWAXMWCAHY-UHFFFAOYSA-N
Formula: C10H15NO
SMILES: Cc1ccc(C=O)n1CC(C)C
Mol. weight [g/mol]: 165.23
CAS: 66054-34-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	2.265		Crippen Method
mcvol	143.850	ml/mol	McGowan Method
ripol	1810.00		NIST Webbook
ripol	1810.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66054340&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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