N-Methylfentanyl

Inchi: InChI=1S/C15H22N2O/c1-3-15(18)17(13-7-5-4-6-8-13)14-9-11-16(2)12-10-14/h4-8,14H,
InchiKey: PCMUWYHREXSXFM-UHFFFAOYSA-N
Formula: C15H22N2O
SMILES: CCC(=O)N(c1ccccc1)C1CCN(C)CC1
Mol. weight [g/mol]: 246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.524		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
rinpol	2018.00		NIST Webbook
rinpol	2018.00		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=R193287&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

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