

1-(4-Ethylpiperazin-1-yl)ethanone

Inchi: InChI=1S/C8H16N2O/c1-3-9-4-6-10(7-5-9)8(2)11/h3-7H2,1-2H3
InchiKey: VUHRYOBNDRCGBH-UHFFFAOYSA-N
Formula: C8H16N2O
SMILES: CCN1CCN(C(C)=O)CC1
Mol. weight [g/mol]: 156.23

Physical Properties

Property code	Value	Unit	Source
log10ws	0.02		Crippen Method
logp	0.170		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U372970&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/59-922-3/1-4-Ethylpiperazin-1-yl-ethanone.pdf>

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