

# 1-(4-Ethylpiperazin-1-yl)-2,2,2-trifluoroethanone

<b>Inchi:</b>	InChI=1S/C8H13F3N2O/c1-2-12-3-5-13(6-4-12)7(14)8(9,10)11/h2-6H2,1H3
<b>InchiKey:</b>	QXUTXTAYZAVQKI-UHFFFAOYSA-N
<b>Formula:</b>	C8H13F3N2O
<b>SMILES:</b>	CCN1CCN(C(=O)C(F)(F)F)CC1
<b>Mol. weight [g/mol]:</b>	210.20

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.64		Crippen Method
logp	0.713		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
rinpola	1231.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U373192&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373192&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/24-762-9/1-4-Ethylpiperazin-1-yl-2-2-2-trifluoroethanone.pdf>

Generated by Cheméo on 2024-04-28 11:34:53.976065858 +0000 UTC m=+16593342.896643173.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.