

Ethanone, 1-(4-phenyl-1-piperazinyl)-

Other names:	Piperazine, 1-phenyl, 4-acetyl
Inchi:	InChI=1S/C12H16N2O/c1-11(15)13-7-9-14(10-8-13)12-5-3-2-4-6-12/h2-6H,7-10H2,1H3
InchiKey:	YFBOBXSXWBMZCY-UHFFFAOYSA-N
Formula:	C12H16N2O
SMILES:	CC(=O)N1CCN(c2ccccc2)CC1
Mol. weight [g/mol]:	204.27
CAS:	21557-13-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	1.355		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
rinpol	1920.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1872.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21557131&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/85-409-4/Ethanone-1-4-phenyl-1-piperazinyl.pdf>

Generated by Cheméo on 2024-04-25 16:36:31.797263174 +0000 UTC m=+16352240.717840486.

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