

Piperazine, 1-acetyl-4-(4-chlorophenoxyacetyl)

Inchi: InChI=1S/C14H17ClN2O3/c1-11(18)16-6-8-17(9-7-16)14(19)10-20-13-4-2-12(15)3-5-13/
InchiKey: GDMDWWIPJXSYMA-UHFFFAOYSA-N
Formula: C14H17ClN2O3
SMILES: CC(=O)N1CCN(C(=O)COc2ccc(Cl)cc2)CC1
Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.79		Crippen Method
logp	1.409		Crippen Method
mcvol	214.710	ml/mol	McGowan Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		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=R408925&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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<https://www.chemeo.com/cid/58-560-6/Piperazine-1-acetyl-4-4-chlorophenoxyacetyl.pdf>

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