# Pyrrobutamine M (oxo), acetylated

**Inchi:** InChI=1S/C20H20ClNO/c21-19-10-8-16(9-11-19)15-18(17-5-2-1-3-6-17)12-14-22-13-4-7
**InchiKey:** ORFURAUSBAEOCC-LDADJPATSA-N
**Formula:** C20H20ClNO
**SMILES:** O=C1CCCN1CC=C(Cc1ccc(Cl)cc1)c1ccccc1
**Mol. weight [g/mol]:** 325.83

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.35 | | Crippen Method |
| logp | 4.588 | | Crippen Method |
| mcvol | 253.770 | ml/mol | McGowan Method |
| rinpol | 2920.00 | | NIST Webbook |
| rinpol | 2920.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R120724&Units=SI
**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

## 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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