# D-p-Chlorophenylalanine, N-dimethylaminomethylene-, butyl ester

**Inchi:** InChI=1S/C16H23ClN2O2/c1-4-5-10-21-16(20)15(18-12-19(2)3)11-13-6-8-14(17)9-7-13/

**InchiKey:** NXXVBSCGDZGHDM-UHFFFAOYSA-N

**Formula:** C16H23ClN2O2

**SMILES:** CCCCOC(=O)C(Cc1ccc(Cl)cc1)N=CN(C)C

**Mol. weight [g/mol]:** 310.82

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -264.58 | kJ/mol | Joback Method |
| hvap | 72.66 | kJ/mol | Joback Method |
| log10ws | -3.51 | | Crippen Method |
| logp | 3.184 | | Crippen Method |
| mcvol | 247.880 | ml/mol | McGowan Method |
| pc | 1564.75 | kPa | Joback Method |
| rinpol | 2174.00 | | NIST Webbook |
| rinpol | 2174.00 | | NIST Webbook |
| tb | 799.54 | K | Joback Method |
| tc | 1013.12 | K | Joback Method |

## Sources

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U375822&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## Legend

**hf:** Enthalpy of formation at standard conditions

**hvap:** Enthalpy of vaporization at standard conditions

| | |
|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |