

# 4-CHLORO-2-PHENYLQUINAZOLINE

|                      |                                                                              |
|----------------------|------------------------------------------------------------------------------|
| Other names:         | 4-Chloro-2-phenylquinazoline<br>Quinazoline, 4-chloro-2-phenyl-              |
| Inchi:               | InChI=1S/C14H9ClN2/c15-13-11-8-4-5-9-12(11)16-14(17-13)10-6-2-1-3-7-10/h1-9H |
| InchiKey:            | OBHKONRNYCDRKM-UHFFFAOYSA-N                                                  |
| Formula:             | C14H9ClN2                                                                    |
| SMILES:              | Clc1nc(-c2ccccc2)nc2ccccc12                                                  |
| Mol. weight [g/mol]: | 240.69                                                                       |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| ie            | 8.47    | eV     | Cheméo Relay (1.0) |
| logp          | 3.950   |        | Crippen Method     |
| mcvol         | 173.340 | ml/mol | McGowan Method     |
| tb            | 647.41  | K      | Cheméo Relay (1.0) |
| tf            | 405.97  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| Cheméo Relay (1.0):       |                                                                                                                                             |
| Cheméo Relay (1.0, beta): |                                                                                                                                             |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6484259&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6484259&amp;Units=SI</a> |

## Legend

|        |                                     |
|--------|-------------------------------------|
| ie:    | Ionization energy                   |
| logp:  | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume     |
| tb:    | Normal Boiling Point Temperature    |

**tf:** Normal melting (fusion) point

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