

1,7-Phenanthroline

InChI:

InChI=1S/C12H8N2/c1-3-9-5-6-11-10(4-2-7-13-11)12(9)14-8-1/h1-8H

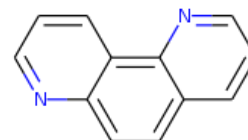
InChI Key: OZKOMUDCMCEDTM-UHFFFAOYSA-N

Formula: C₁₂H₈N₂

SMILES: c1cnc2c(c1)ccc1ncccc12

Molecular Weight: 180.21

CAS: 230-46-6



Physical Properties

Property	Value	Unit	Source
$\Delta_{\text{vap}} H^\circ$	79.40 ± 4.70	kJ/mol	NIST Webbook
$\log P_{\text{oct/wat}}$	2.78		Crippen Method

Sources

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H8N2/c1-3-9-5-6-11-10\(4-2-7-13-11\)12\(9\)14-8-1/h1-8H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H8N2/c1-3-9-5-6-11-10(4-2-7-13-11)12(9)14-8-1/h1-8H)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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