2-Phenyl-4,7-dichloro-quinoline

Inchi: InChI=1S/C15H9Cl2N/c16-11-6-7-12-13(17)9-14(18-15(12)8-11)10-4-2-1-3-5-10/h1-9H
InchiKey: PCHBNMXAFNHKRD-UHFFFAOYSA-N
Formula: C15H9Cl2N
SMILES: Clc1ccc2c(Cl)cc(-c3ccccc3)nc2c1
Mol. weight [g/mol]: 274.15

Physical Properties

Property code	Value	Unit	Source
hvap	102.82	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.11		Cheméo Relay (1.0)
logp	5.209		Crippen Method
mcvol	189.690	ml/mol	McGowan Method
tb	670.56	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116434947&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

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
tb: Normal Boiling Point Temperature

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https://www.chemeo.com/cid/91-248-6/2-Phenyl-4-7-dichloro-quinoline.pdf

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