

Naphtho[2,3-d]-1,2,3-triazin-4(3H)-one, 3-phenyl-

Other names:

Naphtho[2,3-d]-v-triazin-4(3H)-one, 3-phenyl-
3-Phenylnaphtho[2,3-d][1,2,3]triazin-4(3H)-one

Naphtho[2,3-e]-4-hydro-4-oxo-3-phenyl-1,2,3-triazine

Inchi: InChI=1S/C17H11N3O/c21-17-15-10-12-6-4-5-7-13(12)11-16(15)18-19-20(17)14-8-2-1-3

InchiKey: OHHFEIRDCKETFR-UHFFFAOYSA-N

Formula: C17H11N3O

SMILES: O=c1c2cc3ccccc3cc2nnn1-c1cccc1

Mol. weight [g/mol]: 273.29

CAS: 19275-09-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	2.934		Crippen Method
mcvol	199.760	ml/mol	McGowan Method

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C19275093&Units=SI>

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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