

1H-Naphtho[2,3-d][1,2,3]triazole

Other names:	1H-Naphtho[2,3-d]triazole
Inchi:	InChI=1S/C10H7N3/c1-2-4-8-6-10-9(11-13-12-10)5-7(8)3-1/h1-6H,(H,11,12,13)
InchiKey:	NSFXVRRBG NORBD-UHFFFAOYSA-N
Formula:	C10H7N3
SMILES:	c1ccc2cc3[nH]nnc3cc2c1
Mol. weight [g/mol]:	169.18
CAS:	269-12-5

Physical Properties

Property code	Value	Unit	Source
chs	-5209.70 ± 2.00	kJ/mol	NIST Webbook
log10ws	-3.83		Crippen Method
logp	1.629		Crippen Method
mcvol	123.320	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=C269125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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