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: NSFXVRRBGNORBD-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