4-Phenylfurazanamine

Inchi: InChI=1S/C8H7N3O/c9-8-7(10-12-11-8)6-4-2-1-3-5-6/h1-5H,(H2,9,11)
InchiKey: APGIIVSHRRCAPU-UHFFFAOYSA-N
Formula: C8H7N3O
SMILES: Nc1nonc1-c1ccccc1
Mol. weight [g/mol]: 161.16
CAS: 10349-14-1

Physical Properties

Property code	Value	Unit	Source
chs	-4369.40 ± 5.00	kJ/mol	NIST Webbook
log10ws	-6.97		Crippen Method
logp	1.319		Crippen Method
mcvol	116.170	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10349141&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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