3-Methyl-4-phenylfurazan

Inchi: InChI=1S/C9H8N2O/c1-7-9(11-12-10-7)8-5-3-2-4-6-8/h2-6H,1H3
InchiKey: NJFVZLLKYNGWAE-UHFFFAOYSA-N
Formula: C9H8N2O
SMILES: Cc1nonc1-c1ccccc1
Mol. weight [g/mol]: 160.17
CAS: 10349-09-4

Physical Properties

Property code	Value	Unit	Source
chs	-4872.70 ± 5.00	kJ/mol	NIST Webbook
log10ws	-7.82		Crippen Method
logp	2.045		Crippen Method
mcvol	120.280	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=C10349094&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.