

3-Phenylfurazan

Other names:	Phenylfurazan
Inchi:	InChI=1S/C8H6N2O/c1-2-4-7(5-3-1)8-6-9-11-10-8/h1-6H
InchiKey:	CHJJHGSNNPEDNJ-UHFFFAOYSA-N
Formula:	C8H6N2O
SMILES:	c1ccc(-c2cnon2)cc1
Mol. weight [g/mol]:	146.15
CAS:	10349-06-1

Physical Properties

Property code	Value	Unit	Source
chs	-4243.40 ± 4.20	kJ/mol	NIST Webbook
log10ws	-7.34		Crippen Method
logp	1.737		Crippen Method
mcvol	106.190	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10349061&Units=SI

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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