

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:	<chem>c1ccc(-c2cnon2)cc1</chem>
Mol. weight [g/mol]:	146.15

Physical Properties

Property code	Value	Unit	Source
chs	-4243.40 ± 4.20	kJ/mol	NIST Webbook
hf	314.47	kJ/mol	Cheméo Relay (1.0)
hvap	74.46	kJ/mol	Cheméo Relay (1.0)
logp	1.737		Crippen Method
mcvol	106.190	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C10349061&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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