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

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