

1H-Pyrrole, 2-phenyl-

Other names:	Pyrrole, 2-phenyl- 2-Phenylpyrrole
Inchi:	InChI=1S/C10H9N/c1-2-5-9(6-3-1)10-7-4-8-11-10/h1-8,11H
InchiKey:	IRTLROCMFSDSNF-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	<chem>c1ccc(-c2ccc[nH]2)cc1</chem>
Mol. weight [g/mol]:	143.19
CAS:	3042-22-6

Physical Properties

Property code	Value	Unit	Source
chs	-5360.50 ± 5.40	kJ/mol	NIST Webbook
log10ws	-3.29		Crippen Method
logp	2.200		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
tf	403.00 ± 2.00	K	NIST Webbook
tf	403.00 ± 2.00	K	NIST Webbook

Sources

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=C3042226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

tf: Normal melting (fusion) point

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