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: c1ccc(-c2ccc[nH]2)cc1
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/ci990307l

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