2-Phenylbenzoxazole

Other names: 2-phenylbenzo[d]oxazole
Inchi: InChI=1S/C13H9NO/c1-2-6-10(7-3-1)13-14-11-8-4-5-9-12(11)15-13/h1-9H
InchiKey: FIISKTXZUZBTRC-UHFFFAOYSA-N
Formula: C13H9NO
SMILES: c1ccc(-c2nc3ccccc3o2)cc1
Mol. weight [g/mol]: 195.22

Physical Properties

Property code	Value	Unit	Source
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-4.22		Cheméo Relay (1.0)
logp	3.495		Crippen Method
mcvol	147.200	ml/mol	McGowan Method
tb	592.25	K	Cheméo Relay (1.0)
tf	335.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	90.90	kJ/mol	298.15	Thermochemical and conformational study of optical active phenylbenzazole derivatives

Sources

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):

Cheméo Relay (1.0, beta):

Thermochemical and conformational study of optical active phenylbenzazole derivatives:	https://www.doi.org/10.1016/j.jct.2017.08.017
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C833501&Units=SI

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point