1-(2-AMINOPHENYL)PYRROLE

Other names: 1-(2'-Aminophenyl)pyrrole
2-(1H-pyrrol-1-yl)aniline
Benzenamine, 2-(1H-pyrrol-1-yl)-
N-(2-Aminophenyl)pyrrole
Inchi: InChI=1S/C10H10N2/c11-9-5-1-2-6-10(9)12-7-3-4-8-12/h1-8H,11H2
InchiKey: GDMZHPUPLWQIBD-UHFFFAOYSA-N
Formula: C10H10N2
SMILES: Nc1ccccc1-n1cccc1
Mol. weight [g/mol]: 158.20

Physical Properties

Property code	Value	Unit	Source
ie	7.18	eV	Cheméo Relay (1.0)
log10ws	-2.21		Cheméo Relay (1.0)
logp	2.059		Crippen Method
mcvol	128.500	ml/mol	McGowan Method
tb	570.31	K	Cheméo Relay (1.0)
tf	334.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	98.80	kJ/mol	298.15	Energetics of 1-(aminophenyl)pyrroles: A joint calorimetric and computational study

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Energetics of 1-(aminophenyl)pyrroles: A joint calorimetric and computational study:	https://www.doi.org/10.1016/j.jct.2011.04.022
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6025601&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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