

N-phenylanthranilic acid

Other names:	2-(phenylamino)benzoic acid
Inchi:	InChI=1S/C13H11NO2/c15-13(16)11-8-4-5-9-12(11)14-10-6-2-1-3-7-10/h1-9,14H,(H,15,16)H
InchiKey:	ZWJINEZUASEZBH-UHFFFAOYSA-N
Formula:	C13H11NO2
SMILES:	O=C(O)c1cccc1Nc1cccc1
Mol. weight [g/mol]:	213.24

Physical Properties

Property code	Value	Unit	Source
hf	-193.05	kJ/mol	Cheméo Relay (1.0)
hfus	27.91	kJ/mol	Joback Method
hvap	109.26	kJ/mol	Cheméo Relay (1.0)
ie	7.45	eV	Cheméo Relay (1.0)
log10ws	-3.51		Cheméo Relay (1.0)
logp	3.128		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	630.74	K	Cheméo Relay (1.0)
tc	971.99	K	Cheméo Relay (1.0)
tf	442.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.77	J/mol×K	751.40	Joback Method
cpg	448.72	J/mol×K	789.54	Joback Method
cpg	458.76	J/mol×K	827.68	Joback Method
cpg	467.96	J/mol×K	865.82	Joback Method
cpg	476.38	J/mol×K	903.97	Joback Method
cpg	484.07	J/mol×K	942.11	Joback Method
cpg	491.10	J/mol×K	980.25	Joback Method

Sources

Thermochemistry of Drugs.
Experimental and First-Principles
Study of Enthalpies:

<https://www.doi.org/10.1021/je200128y>

McGowan Method:

https://en.wikipedia.org/wiki/Joback_method

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Solubility of N-phenylanthranilic acid in
nine organic solvents from T = (283.15
to 318.15) K: Determination and
modelling:

<https://www.doi.org/10.1016/j.jct.2016.08.017>

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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