Benzoic acid, 2-(phenylamino)-

Other names:	Anthranilic acid, N-phenyl- o-Anilinobenzoic acid Diphenylamine-2-carboxylic acid Fenamic acid N-Phenylanthranilic acid Phenylanthranilic acid 2-(Phenylamino)benzoic acid 2-Anilinobenzoic acid 2-Carboxydiphenylamine Diphenylaminecarboxylic acid-(2) N-Phenyl-o-aminobenzoic acid N-Phenyl-2-aminobenzoic acid NSC 215211 o-(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,15,1
InchiKey:	ZWJINEZUASEZBH-UHFFFAOYSA-N
Formula:	C13H11NO2
SMILES:	O=C(O)c1ccccc1Nc1ccccc1
Mol. weight [g/mol]:	213.23
CAS:	91-40-7

Physical Properties

Property code	Value	Unit	Source
gf	97.42	kJ/mol	Joback Method
hf	-61.40	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hsub	126.00 ± 1.30	kJ/mol	NIST Webbook
hvap	79.61	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.128		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	751.40	K	Joback Method
tc	980.25	K	Joback Method
tf	465.04	K	Joback Method
vc	0.608	m3/kmol	Joback Method

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
hfust	39.70	kJ/mol	458.20	NIST Webbook
hsubt	123.00 ± 1.30	kJ/mol	382.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91407&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
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
vc:	Critical Volume