Benzenamine, N-(phenylmethylene)-

Other names:	Aniline, N-benzylidene-
	Benzalaniline
	Benzaldehyde anil
	Benzylideneaniline
	N-Benzalaniline
	N-Benzylidenaniline
	N-Benzylideneaniline
	M4
	N-Phenylbenzenemethanimine
	N-Phenylbenzylideneimine
	Benzylidene-phenyl-amine
	N-(Phenylmethylene)benzenamine
	NSC 736
Inchi:	InChI=1S/C13H11N/c1-3-7-12(8-4-1)11-14-13-9-5-2-6-10-13/h1-11H
InchiKey:	UVEWQKMPXAHFST-UHFFFAOYSA-N
Formula:	C13H11N
SMILES:	C(=Nc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	181.23
CAS:	538-51-2

Physical Properties

Property code	Value	Unit	Source
chs	-6855.50 ± 7.10	kJ/mol	NIST Webbook
chs	-6872.70 ± 1.10	kJ/mol	NIST Webbook
hf	278.70 ± 2.20	kJ/mol	NIST Webbook
hfs	185.00 ± 2.00	kJ/mol	NIST Webbook
hsub	93.70 ± 0.90	kJ/mol	NIST Webbook
hsub	93.70	kJ/mol	NIST Webbook
hsub	93.70 ± 0.90	kJ/mol	NIST Webbook
hsub	98.10 ± 1.20	kJ/mol	NIST Webbook
hvap	52.40	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
ie	8.25	eV	NIST Webbook
ie	8.27 ± 0.05	eV	NIST Webbook
ie	8.25	eV	NIST Webbook
log10ws	-3.34		Crippen Method
logp	3.437		Crippen Method

mcvol	152.190	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1769.00		NIST Webbook
rinpol	1769.00		NIST Webbook
tb	626.88	K	Joback Method
tc	888.46	K	Joback Method
tf	324.15 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.42	kJ/mol	329.70	NIST Webbook
hsubt	97.40 ± 1.20	kJ/mol	310.00	NIST Webbook
hsubt	85.50 ± 2.10	kJ/mol	293.00	NIST Webbook
hsubt	86.00 ± 2.00	kJ/mol	293.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C538512&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation 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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point