Benzenamine, N,N-diphenyl-

Other names: N,N-Diphenylaniline
N,N-diphenylbenzenamine
triphenylamine
Inchi: InChI=1S/C18H15N/c1-4-10-16(11-5-1)19(17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15H
InchiKey: ODHXBMXNKOYIBV-UHFFFAOYSA-N
Formula: C18H15N
SMILES: c1ccc(N(c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]: 245.32
CAS: 603-34-9

Physical Properties

Property code	Value	Unit	Source
affp	908.90	kJ/mol	NIST Webbook
basg	876.40	kJ/mol	NIST Webbook
chs	-9462.00 ± 3.00	kJ/mol	NIST Webbook
gf	548.69	kJ/mol	Joback Method
hf	327.00 ± 4.20	kJ/mol	NIST Webbook
hfs	235.00 ± 3.00	kJ/mol	NIST Webbook
hfus	27.52	kJ/mol	Joback Method
hsub	92.00	kJ/mol	NIST Webbook
hsub	92.00 ± 3.00	kJ/mol	NIST Webbook
hvap	64.53	kJ/mol	Joback Method
ie	7.00 ± 0.05	eV	NIST Webbook
ie	6.86 ± 0.03	eV	NIST Webbook
ie	6.80 ± 0.05	eV	NIST Webbook
ie	6.75 ± 0.01	eV	NIST Webbook
log10ws	-4.97		Crippen Method
logp	5.156		Crippen Method
mcvol	203.180	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	620.70	K	NIST Webbook
tc	968.00	K	Joback Method
tf	399.90 ± 1.00	K	NIST Webbook
tf	400.70 ± 0.60	K	NIST Webbook
tf	399.00 ± 1.50	K	NIST Webbook

tf	399.65 ± 0.60	K	NIST Webbook
tf	398.95 ± 0.50	K	NIST Webbook
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.68	J/mol×K	923.95	Joback Method
cpg	622.88	J/mol×K	968.00	Joback Method
cpg	535.96	J/mol×K	703.72	Joback Method
cpg	554.28	J/mol×K	747.77	Joback Method
cpg	570.85	J/mol×K	791.81	Joback Method
cpg	585.83	J/mol×K	835.86	Joback Method
cpg	599.39	J/mol×K	879.90	Joback Method
cps	297.50	J/mol×K	298.50	NIST Webbook
hfust	24.89	kJ/mol	400.20	NIST Webbook
hfust	24.89	kJ/mol	400.20	NIST Webbook
hsubt	87.90 ± 1.30	kJ/mol	347.50	NIST Webbook
hvapt	65.20	kJ/mol	556.50	NIST Webbook
hvapt	90.20	kJ/mol	298.00	Study of the Anomalous Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603349&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Study of the Anomalous Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography:	https://www.doi.org/10.1021/je900702t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume