Azobenzene

Other names:	1,2-Diphenyldiazene
	Azobenzeen
	Azobenzen
	Azobenzide
	Azobenzol
	Azobisbenzene
	Azodibenzene
	Azodibenzeneazofume
	Azofume
	Benzene, azobis-
	Benzene, azodi-
	Benzeneazobenzene
	Benzofume
	DIPHENYL DIAZENE
	Diazene, 1,2-diphenyl-
	Diazene, diphenyl-
	Diazobenzene
	Diphenyldiazene
	Diphenyldiimide
	ENT 14,611
	NCI-C02926
	NSC 2102
	USAF EK-704
Inchi:	InChI=1S/C12H10N2/c1-3-7-11(8-4-1)13-14-12-9-5-2-6-10-12/h1-10H
InchiKey:	DMLAVOWQYNRWNQ-UHFFFAOYSA-N
Formula:	C12H10N2
SMILES:	c1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]:	182.22
CAS:	103-33-3

Physical Properties

Property code	Value	Unit	Source
chs	-6525.80	kJ/mol	NIST Webbook
chs	-6468.10 ± 3.80	kJ/mol	NIST Webbook
chs	-6452.00	kJ/mol	NIST Webbook
hf	229.27	kJ/mol	Joback Method

hfs	374.00	kJ/mol	NIST Webbook
hsub	93.84 ± 0.12	kJ/mol	NIST Webbook
hvap	53.53	kJ/mol	Joback Method
ie	8.50 ± 0.05	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-4.45		Estimated Solubility Method
logp	4.102		Crippen Method
mcvol	148.080	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	1591.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1556.00		NIST Webbook
tb	566.20	K	NIST Webbook
tc	947.73	K	Joback Method
tf	340.00 ± 1.00	K	NIST Webbook
tf	341.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	22.37	kJ/mol	340.50	NIST Webbook
hfust	22.39	kJ/mol	342.20	NIST Webbook
sfust	65.59	J/mol×K	340.50	NIST Webbook
sfust	65.40	J/mol×K	342.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64400e+01

Coeff. B	-6.24521e+03
Coeff. C	-3.79130e+01
Temperature range (K), min.	424.56
Temperature range (K), max.	599.10

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1493
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103333&Units=SI

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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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