Azobenzene, (E)-

Other names:	Diazene, diphenyl-, (E)- trans-Azobenzene (E)-Diphenyldiazene Diazene,diphenyl-,(trans)-
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:	17082-12-1

Physical Properties

Property code	Value	Unit	Source
chs	-6471.40	kJ/mol	NIST Webbook
chs	-6466.80	kJ/mol	NIST Webbook
chs	-6462.68 ± 0.88	kJ/mol	NIST Webbook
chs	-6459.90 ± 1.00	kJ/mol	NIST Webbook
chs	-6461.50 ± 3.40	kJ/mol	NIST Webbook
hf	413.60	kJ/mol	NIST Webbook
hf	403.80	kJ/mol	NIST Webbook
hf	402.20 ± 2.70	kJ/mol	NIST Webbook
hf	405.50 ± 1.30	kJ/mol	NIST Webbook
hf	410.60	kJ/mol	NIST Webbook
hfs	310.20 ± 3.40	kJ/mol	NIST Webbook
hfs	311.41	kJ/mol	NIST Webbook
hfs	308.60 ± 1.90	kJ/mol	NIST Webbook
hfs	320.00	kJ/mol	NIST Webbook
hfs	317.00 ± 2.00	kJ/mol	NIST Webbook
hvap	72.80 ± 0.70	kJ/mol	NIST Webbook
ie	8.46	eV	NIST Webbook
ie	8.50 ± 0.05	eV	NIST Webbook
log10ws	-3.51		Crippen Method
logp	4.102		Crippen Method
mcvol	148.080	ml/mol	McGowan Method
pc	4400.00 ± 350.00	kPa	NIST Webbook
rhoc	315.24 ± 14.94	kg/m3	NIST Webbook
rinpol	278.00		NIST Webbook

tb	676.52	K	Joback Method
tc	830.00 ± 3.00	K	NIST Webbook
tf	341.00 ± 1.00	K	NIST Webbook
tf	339.15 ± 0.60	K	NIST Webbook
tf	340.50 ± 0.50	K	NIST Webbook
tf	339.99 ± 0.20	K	NIST Webbook
tf	342.20 ± 1.00	K	NIST Webbook
tt	341.06 ± 0.02	K	NIST Webbook
tt	341.00 ± 2.00	K	NIST Webbook
tt	341.03 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	229.00	J/mol×K	298.15	NIST Webbook
hfust	22.53	kJ/mol	341.10	NIST Webbook
hfust	22.65	kJ/mol	341.90	NIST Webbook
hsubt	94.90 ± 0.80	kJ/mol	308.00	NIST Webbook
hsubt	93.80 ± 1.20	kJ/mol	322.50	NIST Webbook
hsubt	92.10 ± 0.90	kJ/mol	319.50	NIST Webbook
hsubt	96.90 ± 0.80	kJ/mol	308.00	NIST Webbook
hvapt	62.30	kJ/mol	471.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17082121&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs: Standard solid enthalpy of combustion
cps: Solid phase heat capacity
hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rhoc:	Critical density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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