Phthalazine

Other names:	Benzo[d]pyridazine
	«beta»-Phenodiazine
	2,3-Benzodiazine
	2,3-Diazanaphthalene
Inchi:	InChI=1S/C8H6N2/c1-2-4-8-6-10-9-5-7(8)3-1/h1-6H
InchiKey:	LFSXCDWNBUNEEM-UHFFFAOYSA-N
Formula:	C8H6N2
SMILES:	c1ccc2cnncc2c1
Mol. weight [g/mol]:	130.15
CAS:	253-52-1

Physical Properties

Property code	Value	Unit	Source
chs	-4253.20 ± 2.10	kJ/mol	NIST Webbook
chs	-4267.00 ± 17.00	kJ/mol	NIST Webbook
hf	329.90 ± 3.30	kJ/mol	NIST Webbook
hf	345.00 ± 18.00	kJ/mol	NIST Webbook
hfs	261.00 ± 17.00	kJ/mol	NIST Webbook
hfs	247.60 ± 2.30	kJ/mol	NIST Webbook
hsub	82.30 ± 2.30	kJ/mol	NIST Webbook
hsub	81.10 ± 0.40	kJ/mol	NIST Webbook
hsub	82.30 ± 2.30	kJ/mol	NIST Webbook
hsub	83.92 ± 0.68	kJ/mol	NIST Webbook
hsub	84.00	kJ/mol	NIST Webbook
hsub	82.30	kJ/mol	NIST Webbook
ie	9.22 ± 0.01	eV	NIST Webbook
ie	8.68	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-2.81		Crippen Method
logp	1.630		Crippen Method
mcvol	100.320	ml/mol	McGowan Method
rinpol	1437.00		NIST Webbook
tf	364.00 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	13.32	kJ/mol	364.50	NIST Webbook
hfust	13.32	kJ/mol	364.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	462.20	K	3.90	NIST Webbook
tbrp	448.20	K	2.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C253521&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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point