Quinazoline

Other names:	1,3-Diazanaphthalene
	1,3-benzodiazine
	4.5-Benzopyrimidine
	Benzo(e)pyrimidine
	Phenmiazine
Inchi:	InChI=1S/C8H6N2/c1-2-4-8-7(3-1)5-9-6-10-8/h1-6H
InchiKey:	JWVCLYRUEFBMGU-UHFFFAOYSA-N
Formula:	C8H6N2
SMILES:	c1ccc2ncncc2c1
Mol. weight [g/mol]:	130.15
CAS:	253-82-7

Physical Properties

Property code	Value	Unit	Source
chs	-4185.80 ± 8.10	kJ/mol	NIST Webbook
chs	-4172.00 ± 2.10	kJ/mol	NIST Webbook
ea	0.58 ± 0.10	eV	NIST Webbook
hf	243.10 ± 2.70	kJ/mol	NIST Webbook
hf	258.60 ± 8.80	kJ/mol	NIST Webbook
hfs	166.50 ± 2.30	kJ/mol	NIST Webbook
hfs	180.30 ± 8.80	kJ/mol	NIST Webbook
hsub	78.30	kJ/mol	NIST Webbook
hsub	76.60 ± 1.40	kJ/mol	NIST Webbook
hsub	77.60 ± 0.50	kJ/mol	NIST Webbook
hsub	76.60 ± 1.40	kJ/mol	NIST Webbook
hsub	76.60	kJ/mol	NIST Webbook
hsub	78.29 ± 0.54	kJ/mol	NIST Webbook
hvap	58.90 ± 2.00	kJ/mol	NIST Webbook
ie	9.08	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
ie	9.00 ± 0.02	eV	NIST Webbook
ie	9.03 ± 0.03	eV	NIST Webbook
log10ws	-2.81		Crippen Method
logp	1.630		Crippen Method
mcvol	100.320	ml/mol	McGowan Method
rinpol	1239.00		NIST Webbook
rinpol	1239.00		NIST Webbook

rinpol	1201.00		NIST Webbook
rinpol	1201.00		NIST Webbook
tb	516.20	K	NIST Webbook
tf	321.00 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	16.95	kJ/mol	320.90	NIST Webbook
hfust	16.95	kJ/mol	320.90	NIST Webbook
hsubt	77.59	kJ/mol	298.15	NIST Webbook
hvapt	58.90	kJ/mol	298.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds
hvapt	59.60	kJ/mol	298.00	Study of the Anomalous Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography

Sources

Study of the Anomalous Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography:	https://www.doi.org/10.1021/je900702t
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C253827&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds:	https://www.doi.org/10.1021/je900034d

Legend

chs:	Standard solid enthalpy of combustion
ea:	Electron affinity
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point