7,8-Benzoquinoline

Other names: .alpha.-benzoquinoline
.alpha.-naphthoquinoline
4-azaphenanthrene
7,8-benzo[h]quinoline
benzo[h]quinoline
«alpha»-Benzoquinoline
Inchi: InChI=1S/C13H9N/c1-2-6-12-10(4-1)7-8-11-5-3-9-14-13(11)12/h1-9H
InchiKey: WZJYKHNJTSNBHV-UHFFFAOYSA-N
Formula: C13H9N
SMILES: c1ccc2c(c1)ccc1cccnc12
Mol. weight [g/mol]: 179.22

Physical Properties

Property code	Value	Unit	Source
af	0.4486		Cheméo Relay (1.0)
chs	-6551.50 ± 4.10	kJ/mol	NIST Webbook
chs	-6562.04 ± 0.88	kJ/mol	NIST Webbook
hf	250.40 ± 2.30	kJ/mol	NIST Webbook
hf	230.50 ± 5.00	kJ/mol	NIST Webbook
hfs	160.20 ± 1.10	kJ/mol	NIST Webbook
hsub	90.20	kJ/mol	NIST Webbook
hsub	80.80 ± 2.60	kJ/mol	NIST Webbook
hsub	90.20 ± 2.00	kJ/mol	NIST Webbook
hsub	90.20 ± 2.00	kJ/mol	NIST Webbook
hsub	90.20 ± 2.00	kJ/mol	NIST Webbook
hsub	90.20	kJ/mol	NIST Webbook
hsub	90.20 ± 2.00	kJ/mol	NIST Webbook
hvap	81.24	kJ/mol	Cheméo Relay (1.0)
ie	8.04 ± 0.02	eV	NIST Webbook
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	-3.25		Cheméo Relay (1.0)
logp	3.388		Crippen Method
mcvol	141.330	ml/mol	McGowan Method
pc	4098.54	kPa	Cheméo Relay (1.0, beta)
rinpol	301.85		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	301.94		NIST Webbook

rinpol	1805.00		NIST Webbook
rinpol	301.85		NIST Webbook
rinpol	301.94		NIST Webbook
rinpol	301.50		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	302.57		NIST Webbook
rinpol	302.22		NIST Webbook
ss	213.20	J/mol×K	NIST Webbook
ss	213.20	J/mol×K	NIST Webbook
tb	622.25	K	Cheméo Relay (1.0)
tc	913.92	K	Cheméo Relay (1.0)
tf	325.00	K	NIST Webbook
tt	324.10 ± 0.01	K	NIST Webbook
tt	324.10 ± 0.01	K	NIST Webbook
vc	0.540	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	206.36	J/mol×K	298.15	NIST Webbook
cps	206.36	J/mol×K	298.15	NIST Webbook
hfust	14.10	kJ/mol	324.10	NIST Webbook
hfust	14.10	kJ/mol	324.10	NIST Webbook
hfust	14.10	kJ/mol	324.10	NIST Webbook
hfust	14.10	kJ/mol	324.10	NIST Webbook
hfust	14.10	kJ/mol	324.10	NIST Webbook
hsubt	80.80 ± 2.50	kJ/mol	308.00	NIST Webbook
hvapt	59.00 ± 0.30	kJ/mol	522.50	NIST Webbook
hvapt	61.50 ± 0.30	kJ/mol	522.50	NIST Webbook
hvapt	71.70 ± 0.10	kJ/mol	522.50	NIST Webbook
hvapt	71.70 ± 0.10	kJ/mol	522.50	NIST Webbook
hvapt	69.00 ± 0.10	kJ/mol	522.50	NIST Webbook
hvapt	66.50 ± 0.10	kJ/mol	522.50	NIST Webbook
hvapt	64.00 ± 0.10	kJ/mol	522.50	NIST Webbook
hvapt	61.50 ± 0.30	kJ/mol	522.50	NIST Webbook
hvapt	59.00 ± 0.30	kJ/mol	522.50	NIST Webbook
hvapt	64.00 ± 0.10	kJ/mol	522.50	NIST Webbook
hvapt	66.50 ± 0.10	kJ/mol	522.50	NIST Webbook
hvapt	69.00 ± 0.10	kJ/mol	522.50	NIST Webbook
sfust	43.51	J/mol×K	324.10	NIST Webbook
sfust	43.51	J/mol×K	324.10	NIST Webbook

sfust	43.51	J/mol×K	324.10	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	611.20	K	95.90	NIST Webbook
tbrp	611.00	K	95.90	NIST Webbook
tbrp	496.00	K	6.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermodynamic properties of three-ring aza-aromatics. 2. Experimental results for phenanthridine, phenanthridine, and 7,8-benzoquinoline, and mutual validation of experiments and computational methods:	https://www.doi.org/10.1016/j.jct.2009.11.011
Additive scheme for calculation of solvation enthalpies of heterocyclic compounds.:	https://www.doi.org/10.1016/j.tca.2016.03.031
NIST-IUPAC Sublimation/vaporization enthalpy at 298.15 K:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C230273&Units=SI

Legend

af:	Acentric Factor
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
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume