Benzo[h]quinoline

Other names:	.alpha.-benzoquinoline
	.alpha.-naphthoquinoline
	4-azaphenanthrene
	7,8-benzo[h]quinoline
	7,8-benzoquinoline
	«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
CAS:	230-27-3

Physical Properties

Property code	Value	Unit	Source
chs	-6562.04 ± 0.88	kJ/mol	NIST Webbook
chs	-6551.50 ± 4.10	kJ/mol	NIST Webbook
hf	230.50 ± 5.00	kJ/mol	NIST Webbook
hf	250.40 ± 2.30	kJ/mol	NIST Webbook
hfs	160.20 ± 1.10	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
hsub	80.80 ± 2.60	kJ/mol	NIST Webbook
ie	8.30 ± 0.10	eV	NIST Webbook
ie	8.04 ± 0.02	eV	NIST Webbook
log10ws	-4.85		Crippen Method
logp	3.388		Crippen Method
mcvol	141.330	ml/mol	McGowan Method
rinpol	302.22		NIST Webbook
rinpol	301.94		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	301.85		NIST Webbook
rinpol	301.94		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	301.50		NIST Webbook
rinpol	302.57		NIST Webbook

rinpol	301.85		NIST Webbook
rinpol	1755.00		NIST Webbook
ss	213.20	J/mol×K	NIST Webbook
ss	213.20	J/mol×K	NIST Webbook
tf	325.00	K	NIST Webbook
tt	324.10 ± 0.01	K	NIST Webbook

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
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	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
hvapt	71.70 ± 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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C230273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of three-ring aza-aromatics. 2. Experimental results for 1,10-phenanthroline, phenanthridine, and 7,8-benzoquinoline, and mutual validation of experiments and computational methods:	https://www.doi.org/10.1016/j.jct.2009.11.011

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature