Benzo[f]quinoline

Other names:	1-Azaphenanthrene
	5,6-Benzo[f]quinoline
	5,6-Benzoquinoline
	b-Naphthoquinoline
	«beta»-Naphthoquinoline
	Â«betaÂ»-Naphthoquinoline
Inchi:	InChI=1S/C13H9N/c1-2-5-11-10(4-1)7-8-13-12(11)6-3-9-14-13/h1-9H
InchiKey:	HCAUQPZEWLULFJ-UHFFFAOYSA-N
Formula:	C13H9N
SMILES:	c1ccc2c(c1)ccc1ncccc12
Mol. weight [g/mol]:	179.22
CAS:	85-02-9

Physical Properties

Property code	Value	Unit	Source
chs	-6552.50 ± 6.20	kJ/mol	NIST Webbook
hf	233.70 ± 7.40	kJ/mol	NIST Webbook
hsub	83.10 ± 6.20	kJ/mol	NIST Webbook
ie	8.14	eV	NIST Webbook
ie	8.14 ± 0.02	eV	NIST Webbook
ie	8.40 ± 0.10	eV	NIST Webbook
log10ws	-3.36		Aqueous Solubility Prediction Method
logp	3.388		Crippen Method
mcvol	141.330	ml/mol	McGowan Method
rinpol	307.94		NIST Webbook
rinpol	307.94		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	309.25		NIST Webbook
rinpol	306.86		NIST Webbook
rinpol	307.94		NIST Webbook
rinpol	307.30		NIST Webbook
rinpol	306.96		NIST Webbook
rinpol	308.27		NIST Webbook
rinpol	307.30		NIST Webbook
rinpol	306.86		NIST Webbook
rinpol	1807.00		NIST Webbook

rinpol	1800.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tf	364.80 ± 2.00	K	NIST Webbook
tf	367.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	83.10 ± 3.60	kJ/mol	305.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	623.20	K	96.10	NIST Webbook
tbrp	623.00	K	96.10	NIST Webbook
tbrp	485.50 ± 2.50	K	2.90	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85029&Units=SI

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation 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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point