5-Quinolinamine

Other names: Quinoline, 5-amino-
5-Aminoquinoline
5-Quinolylamine
Inchi: InChI=1S/C9H8N2/c10-8-4-1-5-9-7(8)3-2-6-11-9/h1-6H,10H2
InchiKey: XMIAFAKRAAMSGX-UHFFFAOYSA-N
Formula: C9H8N2
SMILES: Nc1cccc2ncccc12
Mol. weight [g/mol]: 144.17
CAS: 611-34-7

Physical Properties

Property code	Value	Unit	Source
chs	-4790.50 ± 1.50	kJ/mol	NIST Webbook
hf	210.60 ± 2.00	kJ/mol	NIST Webbook
hfs	105.60 ± 1.90	kJ/mol	NIST Webbook
hsub	105.00	kJ/mol	NIST Webbook
hsub	105.00 ± 0.70	kJ/mol	NIST Webbook
hsub	103.30 ± 3.40	kJ/mol	NIST Webbook
hsub	105.00 ± 0.70	kJ/mol	NIST Webbook
log10ws	-2.68		Crippen Method
logp	1.817		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
tb	583.20	K	NIST Webbook
tb	583.00	K	NIST Webbook
tf	383.00	K	NIST Webbook
tf	381.15 ± 1.00	K	NIST Webbook
tf	379.00 ± 0.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hsubt	102.90 ± 0.70	kJ/mol	339.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	457.00	K	1.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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