8-Quinolinamine

Other names:	Quinoline, 8-amino- 8-Aminoquinoline 8-Quinolylamine
Inchi:	InChI=1S/C9H8N2/c10-8-5-1-3-7-4-2-6-11-9(7)8/h1-6H,10H2
InchiKey:	WREVVZMUNPAPOV-UHFFFAOYSA-N
Formula:	C9H8N2
SMILES:	Nc1cccc2cccnc12
Mol. weight [g/mol]:	144.17
CAS:	578-66-5

Physical Properties

Property code	Value	Unit	Source
chs	-4779.20 ± 1.60	kJ/mol	NIST Webbook
hf	187.60 ± 2.20	kJ/mol	NIST Webbook
hfs	94.30 ± 2.10	kJ/mol	NIST Webbook
hsub	93.33 ± 0.50	kJ/mol	NIST Webbook
hsub	93.30	kJ/mol	NIST Webbook
hsub	93.30 ± 0.50	kJ/mol	NIST Webbook
log10ws	-2.68		Crippen Method
logp	1.817		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
tf	343.00	K	NIST Webbook
tf	337.65 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	93.00 ± 0.50	kJ/mol	305.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	447.20	K	3.50	NIST Webbook
tbrp	432.50 ± 2.50	K	2.70	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C578665&Units=SI

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
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point