3-Quinolinecarbonitrile

Other names:	3-Cyanoquinoline
	Quinolin-3-carbonitrile
	quinoline-3-carbonitrile
Inchi:	InChI=1S/C10H6N2/c11-6-8-5-9-3-1-2-4-10(9)12-7-8/h1-5,7H
InchiKey:	QZZYYBQGTSGDPP-UHFFFAOYSA-N
Formula:	C10H6N2
SMILES:	N#Cc1cnc2ccccc2c1
Mol. weight [g/mol]:	154.17
CAS:	34846-64-5

Physical Properties

Property code	Value	Unit	Source
hsub	91.30 ± 1.80	kJ/mol	NIST Webbook
hsub	93.20 ± 0.80	kJ/mol	NIST Webbook
log10ws	-3.39		Crippen Method
logp	2.106		Crippen Method
mcvol	119.900	ml/mol	McGowan Method
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	93.40 ± 0.70	kJ/mol	319.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34846645&Units=SI
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

Legend

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