2-Quinolinecarbonitrile

Other names:	Quinaldonitrile
	2-Cyanoquinoline
	quinoline-2-carbonitrile
Inchi:	InChI=1S/C10H6N2/c11-7-9-6-5-8-3-1-2-4-10(8)12-9/h1-6H
InchiKey:	WDXARTMCIRVMAE-UHFFFAOYSA-N
Formula:	C10H6N2
SMILES:	N#Cc1ccc2ccccc2n1
Mol. weight [g/mol]:	154.17
CAS:	1436-43-7

Physical Properties

Property code	Value	Unit	Source
hsub	89.30 ± 3.30	kJ/mol	NIST Webbook
hsub	94.40 ± 0.70	kJ/mol	NIST Webbook
log10ws	-3.39		Crippen Method
logp	2.106		Crippen Method
mcvol	119.900	ml/mol	McGowan Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1436437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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