Quinoline, 5-nitro-

Other names: 5-Nitroquinoline
Inchi: InChI=1S/C9H6N2O2/c12-11(13)9-5-1-4-8-7(9)3-2-6-10-8/h1-6H
InchiKey: NDDZXHOCOKCNBM-UHFFFAOYSA-N
Formula: C9H6N2O2
SMILES: O=[N+]([O-])c1cccc2ncccc12
Mol. weight [g/mol]: 174.16
CAS: 607-34-1

Physical Properties

Property code	Value	Unit	Source
hsub	94.20 ± 0.70	kJ/mol	NIST Webbook
log10ws	-3.69		Crippen Method
logp	2.143		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
rinpol	271.91		NIST Webbook
rinpol	264.98		NIST Webbook
rinpol	271.77		NIST Webbook
rinpol	270.15		NIST Webbook
tf	343.00 ± 3.00	K	NIST Webbook
tf	361.65 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	93.20 ± 0.70	kJ/mol	317.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C607341&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
tf:	Normal melting (fusion) point