

# Quinoline, 5-nitro-

<b>Other names:</b>	5-Nitroquinoline
<b>Inchi:</b>	InChI=1S/C9H6N2O2/c12-11(13)9-5-1-4-8-7(9)3-2-6-10-8/h1-6H
<b>InchiKey:</b>	NDDZXHOCOKCNBM-UHFFFAOYSA-N
<b>Formula:</b>	C9H6N2O2
<b>SMILES:</b>	O=[N+]([O-])c1cccc2ncccc12
<b>Mol. weight [g/mol]:</b>	174.16
<b>CAS:</b>	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	270.15		NIST Webbook
rinpol	271.91		NIST Webbook
rinpol	264.98		NIST Webbook
rinpol	271.77		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

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C607341&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C607341&amp;Units=SI</a>

## Legend

<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpola:</b>	Non-polar retention indices
<b>tf:</b>	Normal melting (fusion) point

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