

Quinoline, 6-nitro-

Other names:	6-Nitroquinoline
Inchi:	InChI=1S/C9H6N2O2/c12-11(13)8-3-4-9-7(6-8)2-1-5-10-9/h1-6H
InchiKey:	SMHPLBXIVNQFBA-UHFFFAOYSA-N
Formula:	C9H6N2O2
SMILES:	O=[N+]([O-])c1ccc2ncccc2c1
Mol. weight [g/mol]:	174.16
CAS:	613-50-3

Physical Properties

Property code	Value	Unit	Source
hsub	103.80 ± 1.00	kJ/mol	NIST Webbook
log10ws	-3.69		Crippen Method
logp	2.143		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
rinpol	282.49		NIST Webbook
rinpol	278.95		NIST Webbook
rinpol	283.16		NIST Webbook
rinpol	281.00		NIST Webbook
rinpol	282.49		NIST Webbook
tf	421.65 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	101.50 ± 1.00	kJ/mol	343.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C613503&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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