Quinoline, 2-methyl-8-nitro-

Other names:	2-Methyl-8-nitroquinoline
	8-Nitroquinaldine
	Quinaldine, 8-nitro-
Inchi:	InChI=1S/C10H8N2O2/c1-7-5-6-8-3-2-4-9(12(13)14)10(8)11-7/h2-6H,1H3
InchiKey:	UHPGVDHXHDPYQP-UHFFFAOYSA-N
Formula:	C10H8N2O2
SMILES:	Cc1ccc2cccc([N+](=O)[O-])c2n1
Mol. weight [g/mol]:	188.18
CAS:	881-07-2

Physical Properties

Property code	Value	Unit	Source
hsub	111.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-4.17		Crippen Method
logp	2.451		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
rinpol	303.84		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	108.30 ± 0.80	kJ/mol	353.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C881072&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

rinpol: Non-polar retention indices