Quinoline, 8-nitro-

Other names:	8-Nitroquinoline
Inchi:	InChI=1S/C9H6N2O2/c12-11(13)8-5-1-3-7-4-2-6-10-9(7)8/h1-6H
InchiKey:	OQHHSGRZCKGLCY-UHFFFAOYSA-N
Formula:	C9H6N2O2
SMILES:	O=[N+]([O-])c1cccc2cccnc12
Mol. weight [g/mol]:	174.16
CAS:	607-35-2

Physical Properties

Property code	Value	Unit	Source
hsub	106.70 ± 0.90	kJ/mol	NIST Webbook
log10ws	-3.69		Crippen Method
logp	2.143		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
rinpol	298.09		NIST Webbook
rinpol	297.78		NIST Webbook
rinpol	298.37		NIST Webbook
rinpol	298.46		NIST Webbook
rinpol	298.09		NIST Webbook
tf	361.65 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	104.30 ± 0.90	kJ/mol	345.00	NIST Webbook

Sources

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

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