

7-Chloro-5-iodo-8-quinolinol

Inchi:	InChI=1S/C9H5ClINO/c10-6-4-7(11)5-2-1-3-12-8(5)9(6)13/h1-4,13H
InchiKey:	JBTWPGVHNYETNF-UHFFFAOYSA-N
Formula:	C9H5ClINO
SMILES:	Oc1c(Cl)cc(I)c2cccnc12
Mol. weight [g/mol]:	305.50
CAS:	35048-13-6

Physical Properties

Property code	Value	Unit	Source
hsub	131.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-4.42		Crippen Method
logp	3.198		Crippen Method
mvol	148.360	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	131.00	kJ/mol	398.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	3.37904e+01
Coeff. B	-1.57727e+04
Temperature range (K), min.	470.79
Temperature range (K), max.	553.84

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35048136&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
pvap:	Vapor pressure

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