5-Iodo-8-quinolinol

Inchi: InChI=1S/C9H6INO/c10-7-3-4-8(12)9-6(7)2-1-5-11-9/h1-5,12H
InchiKey: SUQZNPQQZDQDPJ-UHFFFAOYSA-N
Formula: C9H6INO
SMILES: Oc1ccc(I)c2cccnc12
Mol. weight [g/mol]: 271.05
CAS: 13207-63-1

Physical Properties

Property code	Value	Unit	Source
hsub	119.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-3.74		Crippen Method
logp	2.545		Crippen Method
mcvol	136.120	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	118.80	kJ/mol	378.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	3.24549e+01
Coeff. B	-1.42760e+04
Temperature range (K), min.	443.81
Temperature range (K), max.	525.95

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13207631&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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