Iodoquinol

Other names:

5,7-Diiodo-8-hydroxyquinoline
5,7-Diiodo-8-quinolinol
5,7-Diiodo-oxine
5,7-Diodo-8-quinolinol
8-Hydroxy-5,7-diiodoquinoline
8-Quinolinol, 5,7-diiodo-
Di-Quinol
Diamoebin
Diiodohydroxyquin
Diiodohydroxyquinoline
Diiodoquin
Dijodoxichinoline
Dinoleine
Diodohydroxyquin
Diodoquin
Diodoquine
Diodoxylin
Direxiode
Disoquin
Dyodin
Embequin
Enterodiamoebin
Enterosept
Floraquin
Fluoraquin
Ioquin
Ioquin suspension
Lanodoxin
Meobiquin
Moebiquin
NSC 8704
Quinadome
Rafamebin
SS 578
Searlequin
Searlewuin
Sebaquin
Stanquinate
Yodoxin
Zoaquin

Inchi: InChI=1S/C9H5I2NO/c10-6-4-7(11)9(13)8-5(6)2-1-3-12-8/h1-4,13H
InchiKey: UXZFQZANDVDGMM-UHFFFAOYSA-N
Formula: C9H5I2NO
SMILES: Oc1c(I)cc(I)c2cccnc12
Mol. weight [g/mol]: 396.95
CAS: 83-73-8

Physical Properties

Property code	Value	Unit	Source
chs	-4349.70 ± 1.20	kJ/mol	NIST Webbook
hf	220.30 ± 1.90	kJ/mol	NIST Webbook
hfs	93.50 ± 1.70	kJ/mol	NIST Webbook
hsub	126.80 ± 0.80	kJ/mol	NIST Webbook
hsub	111.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-4.89		Crippen Method
logp	3.150		Crippen Method
mcvol	161.940	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	121.90 ± 0.80	kJ/mol	396.50	NIST Webbook
hsubt	110.90	kJ/mol	413.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.53169e+01
Coeff. B	-1.33320e+04
Temperature range (K), min.	532.65
Temperature range (K), max.	666.42

Sources

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/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=C83738&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
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