1H-Indole-2,3-dione

Other names:	2,3-Dihydro-1H-indole-2,3-dione
	2,3-Dihydroindole-2,3-dione
	2,3-Diketoindoline
	2,3-Dioxo-2,3-dihydroindole
	2,3-Dioxoindoline
	2,3-Ketoindoline
	2,3-indolinedione
	Indole-2,3-dione
	Isatic acid lactam
	Isatine
	Isatinic acid anhydride
	Isotin
	NSC 9262
	Pseudoisatin
	indoline-2,3-dione
	isatin
	o-Aminobenzoylformic anhydride
Inchi:	InChI=1S/C8H5NO2/c10-7-5-3-1-2-4-6(5)9-8(7)11/h1-4H,(H,9,10,11)
InchiKey:	JXDYKVIHCLTXOP-UHFFFAOYSA-N
Formula:	C8H5NO2
SMILES:	O=C1Nc2ccccc2C1=O
Mol. weight [g/mol]:	147.13
CAS:	91-56-5

Physical Properties

Property code	Value	Unit	Source
chs	-3594.50 ± 3.80	kJ/mol	NIST Webbook
gf	30.25	kJ/mol	Joback Method
hf	-127.84	kJ/mol	Joback Method
hfs	-268.20 ± 3.80	kJ/mol	NIST Webbook
hfus	15.80	kJ/mol	Joback Method
hsub	118.80 ± 5.10	kJ/mol	NIST Webbook
hvap	51.81	kJ/mol	Joback Method
ie	8.98 ± 0.05	eV	NIST Webbook
log10ws	-1.39		Crippen Method
logp	0.821		Crippen Method
mcvol	102.080	ml/mol	McGowan Method

pc	5015.69	kPa	Joback Method
rinpol	1712.00		NIST Webbook
rinpol	1712.00		NIST Webbook
tb	609.70	K	Joback Method
tc	879.30	K	Joback Method
tf	474.15 ± 1.00	K	NIST Webbook
tf	473.00 ± 4.00	K	NIST Webbook
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.95	J/mol×K	609.70	Joback Method
cpg	248.95	J/mol×K	654.63	Joback Method
cpg	260.16	J/mol×K	699.57	Joback Method
cpg	270.56	J/mol×K	744.50	Joback Method
cpg	280.12	J/mol×K	789.43	Joback Method
cpg	288.83	J/mol×K	834.36	Joback Method
cpg	296.64	J/mol×K	879.30	Joback Method
hfust	27.82	kJ/mol	475.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamics of solubility of isatin in (PEG 400 + water) mixed solvent systems at T = (298.15 to 338.15) K:	https://www.doi.org/10.1016/j.jct.2014.11.008
Solubility and Thermodynamic Functions of Isatin in Pure Solvents:	https://www.doi.org/10.1021/je500396b
Measurement, Correlation, and Thermodynamics of Solubility of Isatin in Nine Different Green Solvents at (298.15 to 338.15) K:	https://www.doi.org/10.1021/je501036r
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume