1H-Indole-2,3-dione, 5-nitro-

Other names: Indole-2,3-dione, 5-nitro-
Isatin, 5-nitro-
5-Nitroisatin
5-Nitroindole-2,3-dione
5-Nitro-1H-indole-2,3-dione
2,3-dihydro-5-nitroindole-2,3-dione

Inchi: InChI=1S/C8H4N2O4/c11-7-5-3-4(10(13)14)1-2-6(5)9-8(7)12/h1-3H,(H,9,11,12)

InchiKey: UNMYHYODJHKLOC-UHFFFAOYSA-N

Formula: C8H4N2O4

SMILES: O=C1Nc2ccc([N+](=O)[O-])cc2C1=O

Mol. weight [g/mol]: 192.13

CAS: 611-09-6

Physical Properties

Property code	Value	Unit	Source
gf	56.17	kJ/mol	Joback Method
hf	-150.07	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	69.07	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	0.730		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
tb	766.52	K	Joback Method
tc	1055.95	K	Joback Method
tf	528.00 ± 4.00	K	NIST Webbook
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.73	J/mol×K	766.52	Joback Method
cpg	327.10	J/mol×K	814.76	Joback Method
cpg	336.36	J/mol×K	863.00	Joback Method

cpg	344.47	J/mol×K	911.24	Joback Method
cpg	351.38	J/mol×K	959.47	Joback Method
cpg	357.07	J/mol×K	1007.71	Joback Method
cpg	361.49	J/mol×K	1055.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611096&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume