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

Other names:	Indole-2,3-dione, 5-methyl-
	5-Methylisatin
	2,3-Dihydro-5-methylindole-2,3-dione
	5-Methylindole-2,3-dione
	5-Methyl-2,3-indolinedione
	5-methylindole-2,3(1H)-dione
Inchi:	InChI=1S/C9H7NO2/c1-5-2-3-7-6(4-5)8(11)9(12)10-7/h2-4H,1H3,(H,10,11,12)
InchiKey:	VAJCSPZKMVQIAP-UHFFFAOYSA-N
Formula:	C9H7NO2
SMILES:	Cc1ccc2c(c1)C(=O)C(=O)N2
Mol. weight [g/mol]:	161.16
CAS:	608-05-9

Physical Properties

Property code	Value	Unit	Source
gf	29.04	kJ/mol	Joback Method
hf	-159.95	kJ/mol	Joback Method
hfus	18.00	kJ/mol	Joback Method
hvap	54.70	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.130		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
tb	637.56	K	Joback Method
tc	901.55	K	Joback Method
tf	506.30	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.28	J/mol×K	637.56	Joback Method
cpg	295.12	J/mol×K	681.56	Joback Method
cpg	307.13	J/mol×K	725.56	Joback Method

cpg	318.28	J/mol×K	769.56	Joback Method
cpg	328.56	J/mol×K	813.56	Joback Method
cpg	337.92	J/mol×K	857.55	Joback Method
cpg	346.34	J/mol×K	901.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C608059&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

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