2,2-Dihydroxyindan-1,3-dione

Other names:	1H-Indene-1,3(2H)-dione, 2,2-dihydroxy- 1,3-Indandione, 2,2-dihydroxy- Ningidrin Ninhydrin hydrate Triketohydrindene hydrate 2,2-Dihydroxy-1,3-indandione 2,2-Dihydroxy-1H-indene-1,3(2H)-dione 1,2,3-Indantrione, 2-hydrate 1,2,3-Indantrione monohydrate 1H-Indene-1,2,3-trione, 2-hydrate indan-1,2,3-trione
Inchi:	InChI=1S/C9H6O4/c10-7-5-3-1-2-4-6(5)8(11)9(7,12)13/h1-4,12-13H
InchiKey:	FEMOMIGRRWSMCU-UHFFFAOYSA-N
Formula:	C9H6O4
SMILES:	O=C1c2ccccc2C(=O)C1(O)O
Mol. weight [g/mol]:	178.14

Physical Properties

Property code	Value	Unit	Source
hf	-490.83	kJ/mol	Cheméo Relay (1.0)
hfus	11.75	kJ/mol	Joback Method
ie	9.48	eV	Cheméo Relay (1.0)
log10ws	-1.97		Cheméo Relay (1.0)
logp	-0.253		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	5594.19	kPa	Joback Method
tb	560.03	K	Cheméo Relay (1.0)
tc	899.47	K	Cheméo Relay (1.0)
tf	387.47	K	Cheméo Relay (1.0)
vc	0.445	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	328.92	J/mol×K	763.96	Joback Method
cpg	337.96	J/mol×K	801.58	Joback Method
cpg	346.81	J/mol×K	839.21	Joback Method
cpg	355.57	J/mol×K	876.83	Joback Method
cpg	364.33	J/mol×K	914.46	Joback Method
cpg	373.19	J/mol×K	952.08	Joback Method
cpg	382.23	J/mol×K	989.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C485472&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume