

1H-Indene-1,2,3-trione

Other names:	1,2,3-Indantrione 1,2,3-Triketohydrindene 1H-Indene-1,2,3-trione Indantrione
Inchi:	InChI=1S/C9H4O3/c10-7-5-3-1-2-4-6(5)8(11)9(7)12/h1-4H
InchiKey:	WVZWEMOFSIEEMU-UHFFFAOYSA-N
Formula:	C9H4O3
SMILES:	O=c1c(=O)c2ccccc2c1=O
Mol. weight [g/mol]:	160.13

Physical Properties

Property code	Value	Unit	Source
hf	-160.78	kJ/mol	Cheméo Relay (1.0)
hvap	80.66	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	NIST Webbook
log10ws	-2.21		Cheméo Relay (1.0)
logp	-0.204		Crippen Method
mcvol	107.760	ml/mol	McGowan Method
pc	3671.11	kPa	Cheméo Relay (1.0, beta)
tb	564.23	K	Cheméo Relay (1.0)
tc	840.48	K	Cheméo Relay (1.0)
tf	447.43	K	Cheméo Relay (1.0)
vc	0.406	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C938249&Units=SI>

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

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	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

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