1H-Indene-1,3(2H)-dione

Other names:	1,3-Indandione
	1,3-Diketohydrindene
	1,3-Indanedione
	1,3-Indanone
	Diketohydrindene
	Indanedione-(1,3)
	Indandione
	indan-1,3-dione
Inchi:	InChI=1S/C9H6O2/c10-8-5-9(11)7-4-2-1-3-6(7)8/h1-4H,5H2
InchiKey:	UHKAJLSKXBADFT-UHFFFAOYSA-N
Formula:	C9H6O2
SMILES:	O=C1CC(=O)c2ccccc21
Mol. weight [g/mol]:	146.14
CAS:	606-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-49.04	kJ/mol	Joback Method
hf	-186.29	kJ/mol	Joback Method
hfus	8.80	kJ/mol	Joback Method
hsub	97.30 ± 1.80	kJ/mol	NIST Webbook
hvap	47.28	kJ/mol	Joback Method
ie	9.43 ± 0.05	eV	NIST Webbook
log10ws	-2.27		Crippen Method
logp	1.456		Crippen Method
mcvol	106.190	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
rinpol	1358.00		NIST Webbook
rinpol	232.60		NIST Webbook
rinpol	232.00		NIST Webbook
rinpol	232.60		NIST Webbook
rinpol	1358.00		NIST Webbook
tb	584.03	K	Joback Method
tc	844.86	K	Joback Method
tf	403.00 ± 3.00	K	NIST Webbook
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.93	J/mol×K	584.03	Joback Method
cpg	257.77	J/mol×K	627.50	Joback Method
cpg	269.78	J/mol×K	670.97	Joback Method
cpg	280.95	J/mol×K	714.44	Joback Method
cpg	291.28	J/mol×K	757.91	Joback Method
cpg	300.77	J/mol×K	801.38	Joback Method
cpg	309.42	J/mol×K	844.86	Joback Method
hfust	21.80	kJ/mol	401.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C606235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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