1H-Inden-1-one, 2,3-dihydro-

Other names:	1-Indanone
	«alpha»-Hydrindone
	«alpha»-Indanone
	Indan-1-one
	Indanone
	1-Indone
	Indanone-(1)
	2,3-Dihydro-1H-inden-1-one
	2,3-Dihydro-1-indenone
	2,3-Dihydro-1-indanone
Inchi:	InChI=1S/C9H8O/c10-9-6-5-7-3-1-2-4-8(7)9/h1-4H,5-6H2
InchiKey:	QNXSIUBBGPHDDE-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	O=C1CCc2ccccc21
Mol. weight [g/mol]:	132.16
CAS:	83-33-0

Physical Properties

Property code	Value	Unit	Source
gf	73.55	kJ/mol	Joback Method
hf	-48.59	kJ/mol	Joback Method
hfus	9.29	kJ/mol	Joback Method
hsub	83.50 ± 0.70	kJ/mol	NIST Webbook
hsub	78.70 ± 2.80	kJ/mol	NIST Webbook
hvap	43.03	kJ/mol	Joback Method
ie	9.31	eV	NIST Webbook
log10ws	-2.41		Crippen Method
logp	1.816		Crippen Method
mcvol	104.620	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	218.86		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	218.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	218.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1292.00		NIST Webbook

rinpol	1320.00		NIST Webbook
rinpol	216.90		NIST Webbook
ripol	1973.00		NIST Webbook
tb	517.20	K	NIST Webbook
tc	761.48	K	Joback Method
tf	313.00 ± 4.00	K	NIST Webbook
tf	315.15 ± 1.00	K	NIST Webbook
tf	351.00 ± 2.00	K	NIST Webbook
tf	313.00 ± 2.00	K	NIST Webbook
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.20	J/mol×K	516.21	Joback Method
cpg	237.69	J/mol×K	557.09	Joback Method
cpg	250.26	J/mol×K	597.97	Joback Method
cpg	261.96	J/mol×K	638.85	Joback Method
cpg	272.82	J/mol×K	679.73	Joback Method
cpg	282.89	J/mol×K	720.60	Joback Method
cpg	292.23	J/mol×K	761.48	Joback Method
hfust	17.60	kJ/mol	314.10	NIST Webbook
hfust	17.78	kJ/mol	312.90	NIST Webbook
hvapt	60.30 ± 0.40	kJ/mol	333.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	514.70	K	98.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C83330&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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume