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

Other names:	2-Indanone
	1,3-Dihydro-2H-inden-2-one
	«beta»-Hydrindone
	Indanone
	indan-2-one
Inchi:	InChI=1S/C9H8O/c10-9-5-7-3-1-2-4-8(7)6-9/h1-4H,5-6H2
InchiKey:	UMJJFEIKYGFCAT-UHFFFAOYSA-N
Formula:	C9H8O
SMILES:	O=C1Cc2ccccc2C1
Mol. weight [g/mol]:	132.16
CAS:	615-13-4

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	78.30 ± 1.10	kJ/mol	NIST Webbook
hvap	43.03	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.354		Crippen Method
mcvol	104.620	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	516.21	K	Joback Method
tc	761.48	K	Joback Method
tf	331.00 ± 3.00	K	NIST Webbook
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.89	J/mol×K	720.60	Joback Method
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	292.23	J/mol×K	761.48	Joback Method
hfust	16.89	kJ/mol	330.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615134&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
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