2H-Inden-2-one, octahydro-, cis-

Other names:	2-Indanone, hexahydro-, cis- cis-2-Hydrinanone cis-Octahydro-2H-inden-2-one cis-Perhydro-2-indanone Bicyclo[4.3.0]nonan-8-one Octahydro-2H-inden-2-one, (Z)-
Inchi:	InChI=1S/C9H14O/c10-9-5-7-3-1-2-4-8(7)6-9/h7-8H,1-6H2/t7-,8+
InchiKey:	HAMUKWWZXAKCAU-OCAPTIKFSA-N
Formula:	C9H14O
SMILES:	O=C1CC2CCCCC2C1
Mol. weight [g/mol]:	138.21
CAS:	5689-04-3

Physical Properties

Property code	Value	Unit	Source
chl	-5235.30 ± 1.20	kJ/mol	NIST Webbook
gf	-12.49	kJ/mol	Joback Method
hf	-249.60 ± 1.30	kJ/mol	NIST Webbook
hfl	-307.10 ± 1.30	kJ/mol	NIST Webbook
hfus	8.55	kJ/mol	Joback Method
hvap	57.50 ± 0.30	kJ/mol	NIST Webbook
hvap	57.50	kJ/mol	NIST Webbook
ie	9.14 ± 0.08	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	2.156		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	499.43	K	Joback Method
tc	734.32	K	Joback Method
tf	284.73	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.47	J/mol×K	499.43	Joback Method
cpg	296.85	J/mol×K	538.58	Joback Method
cpg	315.07	J/mol×K	577.73	Joback Method
cpg	332.18	J/mol×K	616.87	Joback Method
cpg	348.20	J/mol×K	656.02	Joback Method
cpg	363.18	J/mol×K	695.17	Joback Method
cpg	377.14	J/mol×K	734.32	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5689043&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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