

2H-Inden-2-one, octahydro-3a-methyl-, cis-

Other names:	2-Indanone, hexahydro-3a-methyl-, cis-3a-Methyloctahydro-2H-inden-2-one, (Z)-
Inchi:	InChI=1S/C10H16O/c1-10-5-3-2-4-8(10)6-9(11)7-10/h8H,2-7H2,1H3/t8-,10+/m0/s1
InchiKey:	AMBOSHXMUMOHBF-WCBMZHEXSA-N
Formula:	C10H16O
SMILES:	CC1CCCCC1CC(=O)C2
Mol. weight [g/mol]:	152.23
CAS:	13351-29-6

Physical Properties

Property code	Value	Unit	Source
chs	-5873.80 ± 3.40	kJ/mol	NIST Webbook
gf	-9.56	kJ/mol	Joback Method
hf	-287.00 ± 3.40	kJ/mol	NIST Webbook
hfs	-347.90 ± 3.40	kJ/mol	NIST Webbook
hfus	4.84	kJ/mol	Joback Method
hsub	60.90 ± 0.20	kJ/mol	NIST Webbook
hsub	60.92 ± 0.17	kJ/mol	NIST Webbook
hvap	41.29	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.546		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	522.55	K	Joback Method
tc	763.29	K	Joback Method
tf	319.90	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.27	J/mol×K	522.55	Joback Method
cpg	344.37	J/mol×K	562.67	Joback Method
cpg	363.07	J/mol×K	602.80	Joback Method

cpg	380.54	J/mol×K	642.92	Joback Method
cpg	396.93	J/mol×K	683.04	Joback Method
cpg	412.39	J/mol×K	723.17	Joback Method
cpg	427.09	J/mol×K	763.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13351296&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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

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