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

Other names: 2-Indanone, hexahydro-3a-methyl-, trans-
3a-Methyloctahydro-2H-inden-2-one, (E)-
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-WPRPVWTQSA-N
Formula: C10H16O
SMILES: CC12CCCCC1CC(=O)C2
Mol. weight [g/mol]: 152.23
CAS: 20379-99-1

Physical Properties

Property code	Value	Unit	Source
chl	-5888.20 ± 2.20	kJ/mol	NIST Webbook
gf	-9.56	kJ/mol	Joback Method
hf	-275.20 ± 2.30	kJ/mol	NIST Webbook
hfl	-333.50 ± 2.20	kJ/mol	NIST Webbook
hfus	4.84	kJ/mol	Joback Method
hvap	58.32 ± 0.17	kJ/mol	NIST Webbook
hvap	58.30 ± 0.20	kJ/mol	NIST Webbook
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

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=C20379991&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
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