

4,7-Methano-5H-inden-5-one, octahydro-

Other names:	4,7-Methanoindan-5(4H)-one, tetrahydro- Tricyclo(5,2,1,0(2,6))decanone-8 Tricyclo[5.2.1.0(2,6)]decan-8-one Corodane 8-Ketotricyclo(5.2.1.0(sup2,6))decane 8-Oxotricyclo(5.2.1.0(2,6))decane Tricyclo[5.2.1.0(2,6)]decanone-8 NSC 77098 4,7-Methanoindan-6-one, hexahydro tricyclo[5.2.1.0(2,6)]decane-8-one
Inchi:	InChI=1S/C10H14O/c11-10-5-6-4-9(10)8-3-1-2-7(6)8/h6-9H,1-5H2
InchiKey:	OMIDXVJKZCPKEI-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	O=C1CC2CC1C1CCCC21
Mol. weight [g/mol]:	150.22
CAS:	13380-94-4

Physical Properties

Property code	Value	Unit	Source
gf	73.17	kJ/mol	Joback Method
hf	-195.53	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	41.70	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.012		Crippen Method
mcvol	120.750	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	515.84	K	Joback Method
tc	746.98	K	Joback Method
tf	316.74	K	Joback Method
vc	0.465	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.43	J/mol×K	515.84	Joback Method
cpg	330.08	J/mol×K	554.36	Joback Method
cpg	348.41	J/mol×K	592.89	Joback Method
cpg	365.50	J/mol×K	631.41	Joback Method
cpg	381.43	J/mol×K	669.93	Joback Method
cpg	396.28	J/mol×K	708.46	Joback Method
cpg	410.13	J/mol×K	746.98	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.20	K	4.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13380944&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
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
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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