3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene

Other names:	Steriochemistry unspecified
	4,7-Methano-1H-indene, 3a,4,5,6,7,7a-hexahydro-
	Dihydrodicyclopentadiene
	Tricyclo(5.2.1.0(2,6))dec-3-ene
	Tricyclo(5.2.1.0(2,6))dec-4-ene
	4,7-Methanoindene, 3a,4,5,6,7,7a-hexahydro-
	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene
Inchi:	InChI=1S/C10H14/c1-2-9-7-4-5-8(6-7)10(9)3-1/h1-2,7-10H,3-6H2
InchiKey:	HANKSFAYJLDDKP-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	C1=CC2C3CCC(C3)C2C1
Mol. weight [g/mol]:	134.22
CAS:	4488-57-7

Physical Properties

Property code	Value	Unit	Source
chs	-5912.00 ± 5.90	kJ/mol	NIST Webbook
gf	225.72	kJ/mol	Joback Method
hf	-0.05	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	37.75	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.609		Crippen Method
mcvol	114.880	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1050.50		NIST Webbook
ripol	1252.70		NIST Webbook
tb	447.18	K	Joback Method
tc	663.03	K	Joback Method
tf	249.28	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.68	J/mol×K	447.18	Joback Method
cpg	277.50	J/mol×K	483.15	Joback Method
cpg	295.87	J/mol×K	519.13	Joback Method
cpg	312.91	J/mol×K	555.10	Joback Method
cpg	328.70	J/mol×K	591.08	Joback Method
cpg	343.35	J/mol×K	627.05	Joback Method
cpg	356.95	J/mol×K	663.03	Joback Method
dvisc	0.0004996	Pa×s	249.28	Joback Method
dvisc	0.0006099	Pa×s	282.26	Joback Method
dvisc	0.0007141	Pa×s	315.25	Joback Method
dvisc	0.0008115	Pa×s	348.23	Joback Method
dvisc	0.0009021	Pa×s	381.21	Joback Method
dvisc	0.0009859	Pa×s	414.20	Joback Method
dvisc	0.0010635	Pa×s	447.18	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4488577&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol: Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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