1H-2-Indenone,2,4,5,6,7,7a-hexahydro-3-(1-methyl

Other names: 2,4,5,6,7,7«alpha»-Hexahydro-3-(1-methylethyl)-7«alpha»-methyl-1H-2-indenone
Inchi: InChI=1S/C13H20O/c1-9(2)12-10-6-4-5-7-13(10,3)8-11(12)14/h9H,4-8H2,1-3H3
InchiKey: AFVWSBDXRVPTBE-UHFFFAOYSA-N
Formula: C13H20O
SMILES: CC(C)C1=C2CCCCC2(C)CC1=O
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	31.67	kJ/mol	Joback Method
hf	-257.09	kJ/mol	Joback Method
hfus	8.46	kJ/mol	Joback Method
hvap	49.51	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.492		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1663.00		NIST Webbook
tb	604.54	K	Joback Method
tc	840.70	K	Joback Method
tf	368.75	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.52	J/mol×K	604.54	Joback Method
cpg	472.36	J/mol×K	643.90	Joback Method
cpg	491.03	J/mol×K	683.26	Joback Method
cpg	508.70	J/mol×K	722.62	Joback Method
cpg	525.52	J/mol×K	761.98	Joback Method
cpg	541.63	J/mol×K	801.34	Joback Method
cpg	557.20	J/mol×K	840.70	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=U196695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/54-420-5/1H-2-Indenone-2-4-5-6-7-7a-hexahydro-3-1-methylethyl-7a-methyl.pdf
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