1-H-Indene-1-one-2,4,5,6,7,7a hexahydro-4,4,7a trimethyl

Inchi: InChI=1S/C12H18O/c1-8-6-7-12(2,3)9-4-5-10(13)11(8)9/h4,8,11H,5-7H2,1-3H3
InchiKey: FUUOXSPCJPACFA-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC1CCC(C)(C)C2=CCC(=O)C21
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	19.90	kJ/mol	Joback Method
hf	-260.38	kJ/mol	Joback Method
hfus	11.92	kJ/mol	Joback Method
hvap	46.39	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.958		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1448.00		NIST Webbook
ripol	1951.00		NIST Webbook
ripol	1951.00		NIST Webbook
tb	567.78	K	Joback Method
tc	802.58	K	Joback Method
tf	351.48	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.20	J/mol×K	567.78	Joback Method
cpg	424.37	J/mol×K	606.91	Joback Method
cpg	443.32	J/mol×K	646.05	Joback Method
cpg	461.19	J/mol×K	685.18	Joback Method
cpg	478.11	J/mol×K	724.31	Joback Method
cpg	494.22	J/mol×K	763.45	Joback Method
cpg	509.65	J/mol×K	802.58	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=R440127&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume