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

Inchi: InChI=1S/C12H18O/c1-11(2)7-4-8-12(3)9(11)5-6-10(12)13/h5H,4,6-8H2,1-3H3
InchiKey: GXSVQZVTXJFCJO-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC1(C)CCCC2(C)C(=O)CC=C12
Mol. weight [g/mol]: 178.27
CAS: 60713-96-4

Physical Properties

Property code	Value	Unit	Source
gf	22.12	kJ/mol	Joback Method
hf	-224.80	kJ/mol	Joback Method
hfus	4.55	kJ/mol	Joback Method
hvap	45.55	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.102		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1448.00		NIST Webbook
ripol	1951.00		NIST Webbook
tb	572.69	K	Joback Method
tc	817.44	K	Joback Method
tf	379.62	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.64	J/mol×K	572.69	Joback Method
cpg	421.05	J/mol×K	613.48	Joback Method
cpg	439.21	J/mol×K	654.27	Joback Method
cpg	456.39	J/mol×K	695.06	Joback Method
cpg	472.89	J/mol×K	735.85	Joback Method
cpg	488.99	J/mol×K	776.64	Joback Method
cpg	504.97	J/mol×K	817.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60713964&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
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