1H-Inden-1-one, 2,3-dihydro-5,7-dimethyl-

Other names: 1-Indanone, 5,7-dimethyl-
Inchi: InChI=1S/C11H12O/c1-7-5-8(2)11-9(6-7)3-4-10(11)12/h5-6H,3-4H2,1-2H3
InchiKey: NXOHUHPRFMGJSZ-UHFFFAOYSA-N
Formula: C11H12O
SMILES: Cc1cc(C)c2c(c1)CCC2=O
Mol. weight [g/mol]: 160.21
CAS: 6682-69-5

Physical Properties

Property code	Value	Unit	Source
gf	71.13	kJ/mol	Joback Method
hf	-112.81	kJ/mol	Joback Method
hfus	13.69	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.432		Crippen Method
mcvol	132.800	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	571.93	K	Joback Method
tc	809.66	K	Joback Method
tf	322.00 ± 8.00	K	NIST Webbook
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.18	J/mol×K	571.93	Joback Method
cpg	327.98	J/mol×K	611.55	Joback Method
cpg	341.90	J/mol×K	651.17	Joback Method
cpg	354.97	J/mol×K	690.79	Joback Method
cpg	367.22	J/mol×K	730.42	Joback Method
cpg	378.69	J/mol×K	770.04	Joback Method
cpg	389.41	J/mol×K	809.66	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=C6682695&Units=SI

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