

# 6,12-Methano-7H-benzocycloundecen-14-one

**Inchi:** InChI=1S/C16H16O/c17-16-14-8-2-1-3-9-15(16)11-13-7-5-4-6-12(13)10-14/h4-7,10-11H,  
**InchiKey:** PKYRRPVJFKOFCM-UHFFFAOYSA-N  
**Formula:** C16H16O  
**SMILES:** O=c1c2cc3ccccc3cc1CCCCC2  
**Mol. weight [g/mol]:** 224.30  
**CAS:** 25401-39-2

## Physical Properties

Property code	Value	Unit	Source
chs	-8633.70 ± 6.30	kJ/mol	NIST Webbook
hf	137.00 ± 13.00	kJ/mol	NIST Webbook
hfs	50.90 ± 6.30	kJ/mol	NIST Webbook
ie	8.31 ± 0.03	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-4.62		Crippen Method
logp	3.469		Crippen Method
mcvol	183.790	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C25401392&Units=SI>

## Legend

**chs:** Standard solid enthalpy of combustion  
**hf:** Enthalpy of formation at standard conditions  
**hfs:** Solid phase enthalpy of formation at standard conditions  
**ie:** Ionization energy

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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