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/ci990307l
Crippen Method: 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