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	8.00	eV	NIST Webbook
ie	8.31 ± 0.03	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

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