4,5,6-Trimethyl-2,3-benzoxalene

Inchi: InChI=1S/C15H14O/c1-9-10(2)15-13-7-5-4-6-12(13)8-14(15)16-11(9)3/h4-8H,1-3H3
InchiKey: RQRZTEYZJZHKQR-UHFFFAOYSA-N
Formula: C15H14O
SMILES: Cc1oc2cc3ccccc3c-2c(C)c1C
Mol. weight [g/mol]: 210.27
CAS: 10435-68-4

Physical Properties

Property code	Value	Unit	Source
chs	-7765.90	kJ/mol	NIST Webbook
hf	2.00	kJ/mol	NIST Webbook
hfs	-138.00	kJ/mol	NIST Webbook
hsub	140.00	kJ/mol	NIST Webbook
hsub	139.50	kJ/mol	NIST Webbook
log10ws	-10.46		Crippen Method
logp	4.463		Crippen Method
mcvol	169.700	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10435684&Units=SI
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

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions

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