2,6-Diphenyl-4-thiopyrone

Inchi: InChI=1S/C17H12OS/c18-15-11-16(13-7-3-1-4-8-13)19-17(12-15)14-9-5-2-6-10-14/h1-12
InchiKey: ATWNDGSQGMSBJZ-UHFFFAOYSA-N
Formula: C17H12OS
SMILES: O=c1cc(-c2ccccc2)sc(-c2ccccc2)c1
Mol. weight [g/mol]: 264.34
CAS: 1029-96-5

Physical Properties

Property code	Value	Unit	Source
chs	-9060.00 ± 12.00	kJ/mol	NIST Webbook
log10ws	-5.86		Crippen Method
logp	4.442		Crippen Method
mcvol	201.330	ml/mol	McGowan Method

Sources

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=C1029965&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.