6-pentyl-2H-pyran-2-thione

Inchi: InChI=1S/C10H14OS/c1-2-3-4-6-9-7-5-8-10(12)11-9/h5,7-8H,2-4,6H2,1H3
InchiKey: LWSUSDLRLNLKEA-UHFFFAOYSA-N
Formula: C10H14OS
SMILES: CCCCCc1cccc(=S)o1
Mol. weight [g/mol]: 182.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.11		Crippen Method
logp	3.742		Crippen Method
mcvol	150.220	ml/mol	McGowan Method
rinpol	1665.00		NIST Webbook
ripol	2604.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R422545&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

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices