1,3-Hexanedione, 4,4,5,5,6,6,6-heptafluoro-1-(2-thienyl)-

Other names: Heptafluoro-1-(2-thienyl)-1,3-hexanedione
4,4,5,5,6,6,6-Heptafluoro-1-(2-thienyl)-1,3-hexanedione
Perfluorobutyryl-(2-thenoyl)methane
2-Thenoylperfluorobutyrylmethane

Inchi: InChI=1S/C10H5F7O2S/c11-8(12,9(13,14)10(15,16)17)7(19)4-5(18)6-2-1-3-20-6/h1-3H,4

InchiKey: QHOQGOZSTQAYRH-UHFFFAOYSA-N

Formula: C10H5F7O2S

SMILES: O=C(CC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1cccs1

Mol. weight [g/mol]: 322.20

CAS: 559-94-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	3.723		Crippen Method
mcvol	164.180	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C559944&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

Latest version available from: