Thiophene-2-thiol, S-heptafluorobutyryl-

Inchi: InChI=1S/C8H3F7OS2/c9-6(10,7(11,12)8(13,14)15)5(16)18-4-2-1-3-17-4/h1-3H
InchiKey: VFBUWTDRYRWDDR-UHFFFAOYSA-N
Formula: C8H3F7OS2
SMILES: O=C(Sc1cccs1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 312.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	4.200		Crippen Method
mcvol	150.780	ml/mol	McGowan Method
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook

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=U375542&Units=SI

Legend

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

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