2-(1-Mercaptoethyl)furan

Inchi: InChI=1S/C6H8OS/c1-5(8)6-3-2-4-7-6/h2-5,8H,1H3
InchiKey: PIIMQPHZYYVEMS-UHFFFAOYSA-N
Formula: C6H8OS
SMILES: CC(S)c1ccco1
Mol. weight [g/mol]: 128.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.54		Crippen Method
logp	2.270		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
rinpol	951.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1396.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R169170&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