

2-Phenyl mercapto-3-phenacyl pyrazine

Inchi:	InChI=1S/C18H14N2OS/c21-17(14-7-3-1-4-8-14)13-16-18(20-12-11-19-16)22-15-9-5-2-6
InchiKey:	LKHVCKQOAXGSDE-UHFFFAOYSA-N
Formula:	C18H14N2OS
SMILES:	O=C(Cc1nccnc1Sc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	306.38
CAS:	116659-82-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	4.053		Crippen Method
mcvol	231.080	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=C116659826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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