Cyclo-Met-Pro-diketopiperazine

Inchi: InChI=1S/C10H16N2O2S/c1-15-6-4-7-10(14)12-5-2-3-8(12)9(13)11-7/h7-8H,2-6H2,1H3,
InchiKey: VFVAGPWBFWJBMN-UHFFFAOYSA-N
Formula: C10H16N2O2S
SMILES: CSCCC1NC(=O)C2CCCN2C1=O
Mol. weight [g/mol]: 228.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.22		Crippen Method
logp	0.229		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R225493&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

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