l-Cysteine, N,S-bis(3-cyclopentylpropionyl)-, methyl ester

Inchi: InChI=1S/C20H33NO4S/c1-25-20(24)17(21-18(22)12-10-15-6-2-3-7-15)14-26-19(23)13-

InchiKey: NEJJDJWZYHXFKY-UHFFFAOYSA-N

Formula: C20H33NO4S

SMILES: COC(=O)C(CSC(=O)CCC1CCCC1)N=C(O)CCC1CCCC1

Mol. weight [g/mol]: 383.55

Physical Properties

Property code	Value	Unit	Source
hf	-735.76	kJ/mol	Joback Method
hvap	103.03	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.685		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
tb	1054.80	K	Joback Method
tc	1293.55	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299658&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature