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)NC(=O)CCC1CCCC1

Mol. weight [g/mol]: 383.55

Physical Properties

Property code	Value	Unit	Source
hfus	47.12	kJ/mol	Joback Method
logp	3.845		Crippen Method
mcvol	307.850	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.42	J/mol×K	990.10	Joback Method
cpg	1078.03	J/mol×K	1028.74	Joback Method
cpg	1091.07	J/mol×K	1067.38	Joback Method
cpg	1102.61	J/mol×K	1106.03	Joback Method
cpg	1112.72	J/mol×K	1144.67	Joback Method
cpg	1121.47	J/mol×K	1183.31	Joback Method
cpg	1128.93	J/mol×K	1221.95	Joback Method

Sources

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

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

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume