L-Cysteine, N,S-bis(5-chlorovaleryl)-, methyl ester

Inchi: InChI=1S/C14H23Cl2NO4S/c1-21-14(20)11(17-12(18)6-2-4-8-15)10-22-13(19)7-3-5-9-16

InchiKey: ICIWTKWNAHYPRV-UHFFFAOYSA-N

Formula: C14H23Cl2NO4S

SMILES: COC(=O)C(CSC(=O)CCCCCl)NC(=O)CCCCCl

Mol. weight [g/mol]: 372.31

Physical Properties

Property code	Value	Unit	Source
hfus	52.10	kJ/mol	Joback Method
logp	2.722		Crippen Method
mcvol	269.510	ml/mol	McGowan Method
rinpol	2892.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.45	J/mol×K	897.12	Joback Method
cpg	788.83	J/mol×K	932.43	Joback Method
cpg	799.17	J/mol×K	967.75	Joback Method
cpg	808.49	J/mol×K	1003.06	Joback Method
cpg	816.81	J/mol×K	1038.38	Joback Method
cpg	824.15	J/mol×K	1073.69	Joback Method
cpg	830.53	J/mol×K	1109.01	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299721&Units=SI

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

Legend

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