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
gf	-328.55	kJ/mol	Joback Method
hf	-743.67	kJ/mol	Joback Method
hfus	52.10	kJ/mol	Joback Method
hvap	91.04	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.722		Crippen Method
mcvol	269.510	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
rinpol	2892.00		NIST Webbook
rinpol	2892.00		NIST Webbook
tb	897.12	K	Joback Method
tc	1109.01	K	Joback Method
tf	551.46	K	Joback Method
vc	1.036	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299721&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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