l-Serine, N,O-bis(5-chlorovaleyl), methyl ester

Other names: L-Seine, N,O-bis(5-chlorovaleyl), methyl ester
Inchi: InChI=1S/C14H23Cl2NO5/c1-21-14(20)11(17-12(18)6-2-4-8-15)10-22-13(19)7-3-5-9-16/
InchiKey: AFGCSGILQIJBKA-UHFFFAOYSA-N
Formula: C14H23Cl2NO5
SMILES: COC(=O)C(COC(=O)CCCCCl)NC(=O)CCCCCl
Mol. weight [g/mol]: 356.24

Physical Properties

Property code	Value	Unit	Source
gf	-466.67	kJ/mol	Joback Method
hf	-917.76	kJ/mol	Joback Method
hfus	49.16	kJ/mol	Joback Method
hvap	86.63	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.006		Crippen Method
mcvol	259.030	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
tb	850.76	K	Joback Method
tc	1050.60	K	Joback Method
tf	539.29	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.30	J/mol×K	850.76	Joback Method
cpg	764.50	J/mol×K	884.07	Joback Method
cpg	775.75	J/mol×K	917.37	Joback Method
cpg	786.07	J/mol×K	950.68	Joback Method
cpg	795.45	J/mol×K	983.99	Joback Method
cpg	803.91	J/mol×K	1017.29	Joback Method
cpg	811.46	J/mol×K	1050.60	Joback Method

Sources

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=U299720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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