L-Cysteine, N,S-bis(2-chlorobenzoyl)-, methyl ester

Other names: L-Cysteine,N,O-bis(2-chlorobenzoyl)-, methyl ester
Inchi: InChI=1S/C18H15Cl2NO4S/c1-25-17(23)15(21-16(22)11-6-2-4-8-13(11)19)10-26-18(24)
InchiKey: FLHMCEAYKRLRKK-UHFFFAOYSA-N
Formula: C18H15Cl2NO4S
SMILES: COC(=O)C(CSC(=O)c1ccccc1Cl)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 412.29

Physical Properties

Property code	Value	Unit	Source
gf	-89.31	kJ/mol	Joback Method
hf	-376.11	kJ/mol	Joback Method
hfus	49.77	kJ/mol	Joback Method
hvap	105.82	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	3.838		Crippen Method
mcvol	278.350	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
tb	1051.96	K	Joback Method
tc	1309.88	K	Joback Method
tf	674.42	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.79	J/mol×K	1051.96	Joback Method
cpg	787.37	J/mol×K	1094.95	Joback Method
cpg	792.60	J/mol×K	1137.93	Joback Method
cpg	796.53	J/mol×K	1180.92	Joback Method
cpg	799.23	J/mol×K	1223.91	Joback Method
cpg	800.74	J/mol×K	1266.90	Joback Method
cpg	801.14	J/mol×K	1309.88	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=U299593&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume