l-Cysteine, N,S-bis(O-anisoyl)-, methyl ester

Inchi: InChI=1S/C20H21NO6S/c1-25-16-10-6-4-8-13(16)18(22)21-15(19(23)27-3)12-28-20(24)
InchiKey: ZOLHAAQVQVIVNH-UHFFFAOYSA-N
Formula: C20H21NO6S
SMILES: COC(=O)C(CSC(=O)c1ccccc1OC)NC(=O)c1ccccc1OC
Mol. weight [g/mol]: 403.45

Physical Properties

Property code	Value	Unit	Source
gf	-258.61	kJ/mol	Joback Method
hf	-650.35	kJ/mol	Joback Method
hfus	48.93	kJ/mol	Joback Method
hvap	106.32	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	2.549		Crippen Method
mcvol	293.790	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
tb	1067.70	K	Joback Method
tc	1316.55	K	Joback Method
tf	681.58	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.41	J/mol×K	1067.70	Joback Method
cpg	915.97	J/mol×K	1109.17	Joback Method
cpg	920.63	J/mol×K	1150.65	Joback Method
cpg	923.40	J/mol×K	1192.12	Joback Method
cpg	924.29	J/mol×K	1233.60	Joback Method
cpg	923.30	J/mol×K	1275.07	Joback Method
cpg	920.45	J/mol×K	1316.55	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299757&Units=SI

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