l-Cysteine, N,S-bis(3-trifluoromethylbenzoyl)-, methyl ester

Inchi: InChI=1S/C20H15F6NO4S/c1-31-17(29)15(27-16(28)11-4-2-6-13(8-11)19(21,22)23)10-3

InchiKey: KTBISDVHBDFTHU-UHFFFAOYSA-N

Formula: C20H15F6NO4S

SMILES: COC(=O)C(CSC(=O)c1cccc(C(F)(F)F)c1)NC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 479.39

Physical Properties

Property code	Value	Unit	Source
gf	-1211.79	kJ/mol	Joback Method
hf	-1580.07	kJ/mol	Joback Method
hfus	50.20	kJ/mol	Joback Method
hvap	94.01	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	4.569		Crippen Method
mcvol	292.670	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	2663.00		NIST Webbook
rinpol	2663.00		NIST Webbook
tb	1012.02	K	Joback Method
tc	1244.14	K	Joback Method
tf	645.50	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.76	J/mol×K	1012.02	Joback Method
cpg	914.15	J/mol×K	1050.71	Joback Method
cpg	921.58	J/mol×K	1089.39	Joback Method
cpg	928.19	J/mol×K	1128.08	Joback Method
cpg	934.06	J/mol×K	1166.77	Joback Method
cpg	939.31	J/mol×K	1205.45	Joback Method
cpg	944.04	J/mol×K	1244.14	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=U299704&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume