l-Cysteine, N,S-bis(2,3,4-trifluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C18H11F6NO4S/c1-29-17(27)11(25-16(26)7-2-4-9(19)14(23)12(7)21)6-30-18(

InchiKey: VRQOUSHWGOOMRB-UHFFFAOYSA-N

Formula: C18H11F6NO4S

SMILES: COC(=O)C(CSC(=O)c1ccc(F)c(F)c1F)NC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 451.34

Physical Properties

Property code	Value	Unit	Source
gf	-1272.83	kJ/mol	Joback Method
hf	-1567.17	kJ/mol	Joback Method
hfus	58.29	kJ/mol	Joback Method
hvap	94.80	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	3.366		Crippen Method
mcvol	264.490	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2688.00		NIST Webbook
rinpol	2688.00		NIST Webbook
tb	992.64	K	Joback Method
tc	1218.58	K	Joback Method
tf	668.20	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.19	J/mol×K	992.64	Joback Method
cpg	790.27	J/mol×K	1030.30	Joback Method
cpg	796.11	J/mol×K	1067.95	Joback Method
cpg	800.72	J/mol×K	1105.61	Joback Method
cpg	804.10	J/mol×K	1143.27	Joback Method
cpg	806.28	J/mol×K	1180.92	Joback Method
cpg	807.27	J/mol×K	1218.58	Joback Method

Sources

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=U299635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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