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

Inchi: InChI=1S/C18H15F2NO4S/c1-25-17(23)15(21-16(22)11-4-2-6-13(19)8-11)10-26-18(24)1

InchiKey: GEAAJDUAIDSLKC-UHFFFAOYSA-N

Formula: C18H15F2NO4S

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

Mol. weight [g/mol]: 379.38

Physical Properties

Property code	Value	Unit	Source
gf	-455.07	kJ/mol	Joback Method
hf	-736.85	kJ/mol	Joback Method
hfus	47.53	kJ/mol	Joback Method
hvap	95.42	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	2.810		Crippen Method
mcvol	257.410	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	2901.00		NIST Webbook
rinpol	2901.00		NIST Webbook
tb	975.64	K	Joback Method
tc	1214.43	K	Joback Method
tf	615.76	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.05	J/mol×K	975.64	Joback Method
cpg	771.78	J/mol×K	1015.44	Joback Method
cpg	779.21	J/mol×K	1055.24	Joback Method
cpg	785.40	J/mol×K	1095.03	Joback Method
cpg	790.38	J/mol×K	1134.83	Joback Method
cpg	794.20	J/mol×K	1174.63	Joback Method
cpg	796.90	J/mol×K	1214.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299681&Units=SI
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

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