l-Cysteine, N,S-bis(2,6-difluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C18H13F4NO4S/c1-27-17(25)13(23-16(24)14-9(19)4-2-5-10(14)20)8-28-18(26

InchiKey: REWRVLZXRKXLLA-UHFFFAOYSA-N

Formula: C18H13F4NO4S

SMILES: COC(=O)C(CSC(=O)c1c(F)cccc1F)NC(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 415.36

Physical Properties

Property code	Value	Unit	Source
gf	-863.95	kJ/mol	Joback Method
hf	-1152.01	kJ/mol	Joback Method
hfus	52.91	kJ/mol	Joback Method
hvap	95.11	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	3.088		Crippen Method
mcvol	260.950	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	2984.00		NIST Webbook
tb	984.14	K	Joback Method
tc	1214.74	K	Joback Method
tf	641.98	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.22	J/mol×K	984.14	Joback Method
cpg	781.06	J/mol×K	1022.57	Joback Method
cpg	787.66	J/mol×K	1061.01	Joback Method
cpg	793.03	J/mol×K	1099.44	Joback Method
cpg	797.20	J/mol×K	1137.87	Joback Method
cpg	800.21	J/mol×K	1176.31	Joback Method
cpg	802.07	J/mol×K	1214.74	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=U299666&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