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
hfus	52.91	kJ/mol	Joback Method
logp	3.088		Crippen Method
mcvol	260.950	ml/mol	McGowan Method
rinpol	2984.00		NIST Webbook
rinpol	2984.00		NIST Webbook

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299666&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices