

# L-Cysteine, N,S-bis(4-fluorobenzoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C18H15F2NO4S/c1-25-17(23)15(21-16(22)11-2-6-13(19)7-3-11)10-26-18(24)1
<b>InchiKey:</b>	JQBGTFYUBVJNAH-UHFFFAOYSA-N
<b>Formula:</b>	C18H15F2NO4S
<b>SMILES:</b>	COC(=O)C(CSC(=O)c1ccc(F)cc1)NC(=O)c1ccc(F)cc1
<b>Mol. weight [g/mol]:</b>	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	2927.00		NIST Webbook
tb	975.64	K	Joback Method
tc	1214.43	K	Joback Method
tf	615.76	K	Joback Method
vc	0.983	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

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

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299610&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299610&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/16-958-1/l-Cysteine-N-S-bis-4-fluorobenzoyl-methyl-ester.pdf>

Generated by Cheméo on 2024-05-03 06:25:57.179474297 +0000 UTC m=+17006806.100051608.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.