

L-Cysteine, S-(2-methoxy-2-oxoethyl)-N-[N-[N-(1-oxopropyl)- methyl ester

InChI: InChI=1S/C27H40N4O8S/c1-6-22(32)29-20(13-18-10-8-7-9-11-18)26(36)31-19(12-17(2))
InChIKey: HBIFAJIXPAZQOJ-UHFFFAOYSA-N
Formula: C27H40N4O8S
SMILES: CCC(O)=NC(Cc1ccccc1)C(O)=NC(CC(C)C)C(O)=NCC(O)=NC(CSCC(=O)OC)C(=O)OC
Mol. weight [g/mol]: 580.69
CAS: 35146-63-5

Physical Properties

Property code	Value	Unit	Source
hf	-1152.13	kJ/mol	Joback Method
hvap	181.84	kJ/mol	Joback Method
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	-3.86		Crippen Method
logp	3.696		Crippen Method
mcvol	444.960	ml/mol	McGowan Method
pc	880.52	kPa	Joback Method
tb	1738.40	K	Joback Method
tc	2612.23	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C35146635&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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