

# D-Cysteine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi:	InChI=1S/C14H25NO6S/c1-6-19-13(17)15-11(8-22-14(18)20-7-2)12(16)21-10(5)9(3)4/h9
InchiKey:	PAEBNKSIBBNKLW-NFJWQWPMSA-N
Formula:	C14H25NO6S
SMILES:	CCOC(=O)NC(CSC(=O)OCC)C(=O)OC(C)C(C)C
Mol. weight [g/mol]:	335.42

## Physical Properties

Property code	Value	Unit	Source
gf	-519.57	kJ/mol	Joback Method
hf	-987.19	kJ/mol	Joback Method
hfus	39.04	kJ/mol	Joback Method
hvap	86.31	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.579		Crippen Method
mvol	256.770	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2066.10		NIST Webbook
rinpol	2066.10		NIST Webbook
tb	866.22	K	Joback Method
tc	1073.72	K	Joback Method
tf	506.08	K	Joback Method
vc	0.963	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.30	J/molxK	866.22	Joback Method
cpg	799.18	J/molxK	900.80	Joback Method
cpg	810.83	J/molxK	935.39	Joback Method
cpg	821.24	J/molxK	969.97	Joback Method
cpg	830.39	J/molxK	1004.55	Joback Method
cpg	838.26	J/molxK	1039.14	Joback Method
cpg	844.85	J/molxK	1073.72	Joback Method

# Sources

<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=R501816&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R501816&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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

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