

# 1,3-Di-(5-carbomethoxyamyl) urea

<b>Inchi:</b>	InChI=1S/C15H28N2O5/c1-21-13(18)9-5-3-7-11-16-15(20)17-12-8-4-6-10-14(19)22-2/h3
<b>InchiKey:</b>	FJBAZZHIYLSVFU-UHFFFAOYSA-N
<b>Formula:</b>	C15H28N2O5
<b>SMILES:</b>	COC(=O)CCCCCNC(=O)NCCCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	316.39
<b>CAS:</b>	6621-60-9

## Physical Properties

Property code	Value	Unit	Source
gf	-342.56	kJ/mol	Joback Method
hf	-848.17	kJ/mol	Joback Method
hfus	51.98	kJ/mol	Joback Method
hvap	86.91	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	1.752		Crippen Method
mcvol	258.620	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
tb	849.39	K	Joback Method
tc	1044.30	K	Joback Method
tf	558.38	K	Joback Method
vc	1.000	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.87	J/mol×K	849.39	Joback Method
cpg	828.78	J/mol×K	881.87	Joback Method
cpg	841.70	J/mol×K	914.36	Joback Method
cpg	853.63	J/mol×K	946.84	Joback Method
cpg	864.57	J/mol×K	979.33	Joback Method
cpg	874.55	J/mol×K	1011.81	Joback Method
cpg	883.56	J/mol×K	1044.30	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=C6621609&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6621609&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>hvap:</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>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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