

# 3-Carbethoxy-2,5-piperazinedione

<b>Inchi:</b>	InChI=1S/C7H10N2O4/c1-2-13-7(12)5-6(11)8-3-4(10)9-5/h5H,2-3H2,1H3,(H,8,11)(H,9,10)
<b>InchiKey:</b>	JGDBWGPUIUGDQTO-UHFFFAOYSA-N
<b>Formula:</b>	C7H10N2O4
<b>SMILES:</b>	CCOC(=O)C1NC(=O)CNC1=O
<b>Mol. weight [g/mol]:</b>	186.17
<b>CAS:</b>	86750-34-7

## Physical Properties

Property code	Value	Unit	Source
gf	-271.17	kJ/mol	Joback Method
hf	-578.07	kJ/mol	Joback Method
hfus	26.71	kJ/mol	Joback Method
hvap	62.77	kJ/mol	Joback Method
log10ws	0.45		Crippen Method
logp	-1.836		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
tb	688.14	K	Joback Method
tc	938.95	K	Joback Method
tf	594.69	K	Joback Method
vc	0.472	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.14	J/molxK	688.14	Joback Method
cpg	369.76	J/molxK	729.94	Joback Method
cpg	383.33	J/molxK	771.74	Joback Method
cpg	395.74	J/molxK	813.55	Joback Method
cpg	406.87	J/molxK	855.35	Joback Method
cpg	416.59	J/molxK	897.15	Joback Method
cpg	424.78	J/molxK	938.95	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C86750347&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C86750347&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>
<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>

# 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>m cvol:</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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