

# Pro, methyl ester

<b>Inchi:</b>	InChI=1S/C6H11NO2/c1-9-6(8)5-3-2-4-7-5/h5,7H,2-4H2,1H3
<b>InchiKey:</b>	BLWYXBNNBYXPPL-UHFFFAOYSA-N
<b>Formula:</b>	C6H11NO2
<b>SMILES:</b>	COC(=O)C1CCCN1
<b>Mol. weight [g/mol]:</b>	129.16

## Physical Properties

Property code	Value	Unit	Source
gf	-110.02	kJ/mol	Joback Method
hf	-313.68	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	45.12	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	-0.089		Crippen Method
mcvol	101.960	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	1243.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1261.00		NIST Webbook
tb	476.80	K	Joback Method
tc	692.67	K	Joback Method
tf	345.47	K	Joback Method
vc	0.373	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.08	J/molxK	476.80	Joback Method
cpg	232.24	J/molxK	512.78	Joback Method
cpg	244.80	J/molxK	548.76	Joback Method
cpg	256.74	J/molxK	584.73	Joback Method
cpg	268.08	J/molxK	620.71	Joback Method
cpg	278.82	J/molxK	656.69	Joback Method
cpg	288.95	J/molxK	692.67	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=R535874&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R535874&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>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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