

# Pentedrone

<b>Inchi:</b>	InChI=1S/C12H17NO/c1-3-7-11(13-2)12(14)10-8-5-4-6-9-10/h4-6,8-9,11,13H,3,7H2,1-2H
<b>InchiKey:</b>	WLIWIUNEJRETFX-UHFFFAOYSA-N
<b>Formula:</b>	C12H17NO
<b>SMILES:</b>	CCCC(NC)C(=O)c1ccccc1
<b>Mol. weight [g/mol]:</b>	191.27
<b>CAS:</b>	879722-57-3

## Physical Properties

Property code	Value	Unit	Source
gf	120.60	kJ/mol	Joback Method
hf	-118.87	kJ/mol	Joback Method
hfus	24.05	kJ/mol	Joback Method
hvap	57.38	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.257		Crippen Method
mvol	167.730	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	1508.40		NIST Webbook
rinpol	1508.40		NIST Webbook
tb	604.24	K	Joback Method
tc	816.64	K	Joback Method
tf	339.01	K	Joback Method
vc	0.634	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.45	J/molxK	604.24	Joback Method
cpg	436.03	J/molxK	639.64	Joback Method
cpg	450.64	J/molxK	675.04	Joback Method
cpg	464.30	J/molxK	710.44	Joback Method
cpg	477.08	J/molxK	745.84	Joback Method
cpg	489.00	J/molxK	781.24	Joback Method
cpg	500.11	J/molxK	816.64	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C879722573&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C879722573&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvpap:</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>rinppl:</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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