

# 2,6-Adamantandione

<b>Inchi:</b>	InChI=1S/C10H12O2/c11-9-5-1-6-3-8(9)4-7(2-5)10(6)12/h5-8H,1-4H2
<b>InchiKey:</b>	UBIAKEDDKXHXTB-UHFFFAOYSA-N
<b>Formula:</b>	C10H12O2
<b>SMILES:</b>	O=C1C2CC3CC1CC(C2)C3=O
<b>Mol. weight [g/mol]:</b>	164.20

## Physical Properties

Property code	Value	Unit	Source
gf	-49.42	kJ/mol	Joback Method
hf	-333.23	kJ/mol	Joback Method
hfus	14.05	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.191		Crippen Method
mvol	122.320	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1498.00		NIST Webbook
tb	583.66	K	Joback Method
tc	829.88	K	Joback Method
tf	384.96	K	Joback Method
vc	0.471	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.99	J/mol×K	583.66	Joback Method
cpg	361.57	J/mol×K	624.70	Joback Method
cpg	378.93	J/mol×K	665.73	Joback Method
cpg	395.12	J/mol×K	706.77	Joback Method
cpg	410.19	J/mol×K	747.81	Joback Method
cpg	424.18	J/mol×K	788.85	Joback Method
cpg	437.16	J/mol×K	829.88	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R44334&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R44334&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>

# 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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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