

# 2,2-Dinitroadamantane

<b>Inchi:</b>	InChI=1S/C10H14N2O4/c13-11(14)10(12(15)16)8-2-6-1-7(4-8)5-9(10)3-6/h6-9H,1-5H2
<b>InchiKey:</b>	LLYKIMPMZLMAOC-UHFFFAOYSA-N
<b>Formula:</b>	C10H14N2O4
<b>SMILES:</b>	O=[N+]([O-])C1([N+](=O)[O-])C2CC3CC(C2)CC1C3
<b>Mol. weight [g/mol]:</b>	226.23
<b>CAS:</b>	88381-75-3

## Physical Properties

Property code	Value	Unit	Source
chs	-5685.20 ± 1.10	kJ/mol	NIST Webbook
gf	253.66	kJ/mol	Joback Method
hf	-154.30 ± 1.80	kJ/mol	NIST Webbook
hfs	-250.70 ± 1.10	kJ/mol	NIST Webbook
hfus	32.53	kJ/mol	Joback Method
hsub	96.40 ± 1.40	kJ/mol	NIST Webbook
hsub	96.40 ± 1.40	kJ/mol	NIST Webbook
hvap	69.18	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	1.692		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	747.27	K	Joback Method
tc	1021.58	K	Joback Method
tf	555.40	K	Joback Method
vc	0.619	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.30	J/mol×K	747.27	Joback Method
cpg	516.00	J/mol×K	792.99	Joback Method
cpg	532.08	J/mol×K	838.71	Joback Method
cpg	547.91	J/mol×K	884.43	Joback Method
cpg	563.86	J/mol×K	930.14	Joback Method

cpg	580.32	J/mol×K	975.86	Joback Method
cpg	597.66	J/mol×K	1021.58	Joback Method
hfust	5.06	kJ/mol	491.20	NIST Webbook

## 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=C88381753&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88381753&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation 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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