

# 1-Adamantanethiol

<b>Other names:</b>	Tricyclo[3.3.1.1
<b>Inchi:</b>	InChI=1S/C10H16S/c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9,11H,1-6H2
<b>InchiKey:</b>	ADJLJNODXLXTIH-UHFFFAOYSA-N
<b>Formula:</b>	C10H16S
<b>SMILES:</b>	SC12CC3CC(CC(C3)C1)C2
<b>Mol. weight [g/mol]:</b>	168.30
<b>CAS:</b>	34301-54-7

## Physical Properties

Property code	Value	Unit	Source
gf	219.66	kJ/mol	Joback Method
hf	-4.11	kJ/mol	Joback Method
hfus	12.78	kJ/mol	Joback Method
hvap	43.04	kJ/mol	Joback Method
ie	8.78	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-3.15		Crippen Method
logp	2.885		Crippen Method
mcvol	135.530	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	511.12	K	Joback Method
tc	758.94	K	Joback Method
tf	308.88	K	Joback Method
vc	0.509	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.46	J/mol×K	511.12	Joback Method
cpg	353.30	J/mol×K	552.42	Joback Method
cpg	372.24	J/mol×K	593.73	Joback Method
cpg	389.57	J/mol×K	635.03	Joback Method
cpg	405.55	J/mol×K	676.33	Joback Method
cpg	420.47	J/mol×K	717.63	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=C34301547&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C34301547&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>

## 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>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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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