

# Adamantane-1-carboxylic acid, butyl ester

Inchi:	InChI=1S/C15H24O2/c1-2-3-4-17-14(16)15-8-11-5-12(9-15)7-13(6-11)10-15/h11-13H,2-
InchiKey:	GUMRTIDEFRAFTH-UHFFFAOYSA-N
Formula:	C15H24O2
SMILES:	CCCCOC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	236.35

## Physical Properties

Property code	Value	Unit	Source
gf	-1.55	kJ/mol	Joback Method
hf	-390.59	kJ/mol	Joback Method
hfus	24.47	kJ/mol	Joback Method
hvap	56.59	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.546		Crippen Method
mcvol	197.070	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1723.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1737.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1714.00		NIST Webbook
ripol	2138.00		NIST Webbook
tb	638.95	K	Joback Method
tc	850.55	K	Joback Method
tf	400.93	K	Joback Method
vc	0.759	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.82	J/molxK	638.95	Joback Method
cpg	601.01	J/molxK	674.22	Joback Method
cpg	620.06	J/molxK	709.48	Joback Method
cpg	638.15	J/molxK	744.75	Joback Method

cpg	655.43	J/mol×K	780.02	Joback Method
cpg	672.09	J/mol×K	815.28	Joback Method
cpg	688.29	J/mol×K	850.55	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=R304759&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R304759&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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