

# 1-Adamantanecarboxylic acid, 2-naphthyl ester

Inchi:	InChI=1S/C21H22O2/c22-20(21-11-14-7-15(12-21)9-16(8-14)13-21)23-19-6-5-17-3-1-2-4
InchiKey:	NDCDEBASC FYTSY-UHFFFAOYSA-N
Formula:	C21H22O2
SMILES:	O=C(Oc1ccc2ccccc2c1)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	306.40

## Physical Properties

Property code	Value	Unit	Source
gf	258.40	kJ/mol	Joback Method
hf	-98.30	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	74.53	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.962		Crippen Method
mvol	238.390	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
tb	826.87	K	Joback Method
tc	1080.23	K	Joback Method
tf	540.19	K	Joback Method
vc	0.909	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.17	J/mol×K	826.87	Joback Method
cpg	789.81	J/mol×K	869.10	Joback Method
cpg	810.05	J/mol×K	911.32	Joback Method
cpg	830.27	J/mol×K	953.55	Joback Method
cpg	850.80	J/mol×K	995.78	Joback Method
cpg	872.03	J/mol×K	1038.00	Joback Method
cpg	894.29	J/mol×K	1080.23	Joback Method

# Sources

<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=U307666&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307666&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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