

# N-(1-nitro-2-naphthyl) acetamid

<b>Inchi:</b>	InChI=1S/C12H10N2O3/c1-8(15)13-11-7-6-9-4-2-3-5-10(9)12(11)14(16)17/h2-7H,1H3,(H
<b>InchiKey:</b>	ZDOWETIOQWADNW-UHFFFAOYSA-N
<b>Formula:</b>	C12H10N2O3
<b>SMILES:</b>	CC(=O)Nc1ccc2ccccc2c1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	230.22
<b>CAS:</b>	5419-82-9

## Physical Properties

Property code	Value	Unit	Source
gf	245.98	kJ/mol	Joback Method
hf	43.78	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	77.32	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.706		Crippen Method
mcvol	165.690	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
tb	785.46	K	Joback Method
tc	1041.85	K	Joback Method
tf	555.36	K	Joback Method
vc	0.644	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.69	J/molxK	785.46	Joback Method
cpg	459.59	J/molxK	828.19	Joback Method
cpg	469.57	J/molxK	870.92	Joback Method
cpg	478.74	J/molxK	913.66	Joback Method
cpg	487.19	J/molxK	956.39	Joback Method
cpg	495.01	J/molxK	999.12	Joback Method
cpg	502.32	J/molxK	1041.85	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=C5419829&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5419829&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>
<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>

# 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>m cvol:</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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