

# 3-Nitroacenaphthene

<b>Inchi:</b>	InChI=1S/C12H9NO2/c14-13(15)11-7-5-9-3-1-2-8-4-6-10(11)12(8)9/h1-3,5,7H,4,6H2
<b>InchiKey:</b>	WTRQPBAHQILXND-UHFFFAOYSA-N
<b>Formula:</b>	C12H9NO2
<b>SMILES:</b>	O=[N+]([O-])c1ccc2cccc3c2c1CC3
<b>Mol. weight [g/mol]:</b>	199.21
<b>CAS:</b>	3807-77-0

## Physical Properties

Property code	Value	Unit	Source
gf	356.44	kJ/mol	Joback Method
hf	190.72	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	64.85	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	2.847		Crippen Method
mvol	143.280	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	693.54	K	Joback Method
tc	959.27	K	Joback Method
tf	490.99	K	Joback Method
vc	0.570	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.23	J/mol×K	693.54	Joback Method
cpg	381.05	J/mol×K	737.83	Joback Method
cpg	391.92	J/mol×K	782.12	Joback Method
cpg	402.01	J/mol×K	826.41	Joback Method
cpg	411.52	J/mol×K	870.69	Joback Method
cpg	420.60	J/mol×K	914.98	Joback Method
cpg	429.44	J/mol×K	959.27	Joback Method

# Sources

<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>
<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=C3807770&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3807770&amp;Units=SI</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>mccvol:</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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