

# 1-Naphthoic acid, 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C20H22O2/c1-4-5-11-17(14-15(2)3)22-20(21)19-13-8-10-16-9-6-7-12-18(16)19
InchiKey:	FTLGLKKAVPEDNW-UHFFFAOYSA-N
Formula:	C20H22O2
SMILES:	CCC#CC(CC(C)C)OC(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	294.39

## Physical Properties

Property code	Value	Unit	Source
gf	290.95	kJ/mol	Joback Method
hf	-23.06	kJ/mol	Joback Method
hfus	37.09	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	4.825		Crippen Method
mcvol	248.280	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	792.05	K	Joback Method
tc	1025.31	K	Joback Method
tf	535.06	K	Joback Method
vc	0.944	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.45	J/molxK	792.05	Joback Method
cpg	726.22	J/molxK	830.93	Joback Method
cpg	741.79	J/molxK	869.80	Joback Method
cpg	756.25	J/molxK	908.68	Joback Method
cpg	769.67	J/molxK	947.56	Joback Method
cpg	782.13	J/molxK	986.44	Joback Method
cpg	793.72	J/molxK	1025.31	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U308823&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308823&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>rinpola:</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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