

# 1-Naphthoic acid, 8-chlorooctyl ester

<b>Inchi:</b>	InChI=1S/C19H23ClO2/c20-14-7-3-1-2-4-8-15-22-19(21)18-13-9-11-16-10-5-6-12-17(16)
<b>InchiKey:</b>	CAPWQQHRUYOIBH-UHFFFAOYSA-N
<b>Formula:</b>	C19H23ClO2
<b>SMILES:</b>	O=C(OCCCCCCCCCl)c1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	318.84

## Physical Properties

Property code	Value	Unit	Source
gf	72.68	kJ/mol	Joback Method
hf	-279.90	kJ/mol	Joback Method
hfus	42.62	kJ/mol	Joback Method
hvap	76.01	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.576		Crippen Method
mcvol	255.030	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinqol	2749.00		NIST Webbook
tb	798.48	K	Joback Method
tc	1011.57	K	Joback Method
tf	477.61	K	Joback Method
vc	0.987	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.38	J/molxK	798.48	Joback Method
cpg	795.54	J/molxK	976.05	Joback Method
cpg	783.85	J/molxK	940.54	Joback Method
cpg	771.35	J/molxK	905.02	Joback Method
cpg	757.98	J/molxK	869.51	Joback Method
cpg	743.68	J/molxK	833.99	Joback Method
cpg	806.49	J/molxK	1011.57	Joback Method
dvisc	0.0001438	Paxs	798.48	Joback Method
dvisc	0.0001772	Paxs	745.00	Joback Method

dvisc	0.0002255	Paxs	691.52	Joback Method
dvisc	0.0002989	Paxs	638.05	Joback Method
dvisc	0.0004171	Paxs	584.57	Joback Method
dvisc	0.0006224	Paxs	531.09	Joback Method
dvisc	0.0010158	Paxs	477.61	Joback Method

## Sources

<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=U355694&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355694&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>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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