

# Hydratropic acid, undec-2-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C20H30O2/c1-3-4-5-6-7-8-9-10-14-17-22-20(21)18(2)19-15-12-11-13-16-19/h1
<b>InchiKey:</b>	MGGBVIFSTADQDO-GXDHUFHOSA-N
<b>Formula:</b>	C20H30O2
<b>SMILES:</b>	CCCCCCCCC=CCOC(=O)C(C)c1cccc1
<b>Mol. weight [g/mol]:</b>	302.45

## Physical Properties

Property code	Value	Unit	Source
gf	73.79	kJ/mol	Joback Method
hf	-352.46	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.640		Crippen Method
mcvol	272.040	ml/mol	McGowan Method
pc	1370.73	kPa	Joback Method
rinsol	2180.00		NIST Webbook
tb	763.69	K	Joback Method
tc	961.75	K	Joback Method
tf	393.66	K	Joback Method
vc	1.046	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.49	J/molxK	763.69	Joback Method
cpg	820.54	J/molxK	796.70	Joback Method
cpg	837.52	J/molxK	829.71	Joback Method
cpg	853.49	J/molxK	862.72	Joback Method
cpg	868.49	J/molxK	895.73	Joback Method
cpg	882.58	J/molxK	928.74	Joback Method
cpg	895.79	J/molxK	961.75	Joback Method
dvisc	0.0014700	Paxs	393.66	Joback Method
dvisc	0.0005990	Paxs	455.33	Joback Method

dvisc	0.0003024	Paxs	517.00	Joback Method
dvisc	0.0001766	Paxs	578.67	Joback Method
dvisc	0.0001144	Paxs	640.35	Joback Method
dvisc	0.0000800	Paxs	702.02	Joback Method
dvisc	0.0000592	Paxs	763.69	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406960&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406960&amp;Units=SI</a>
<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>

## 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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