

# Hydratropic acid, dodecyl ester

<b>Inchi:</b>	InChI=1S/C21H34O2/c1-3-4-5-6-7-8-9-10-11-15-18-23-21(22)19(2)20-16-13-12-14-17-20
<b>InchiKey:</b>	ITGFNTHMLVDKAR-UHFFFAOYSA-N
<b>Formula:</b>	C21H34O2
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C(C)c1cccc1
<b>Mol. weight [g/mol]:</b>	318.49

## Physical Properties

Property code	Value	Unit	Source
gf	1.99	kJ/mol	Joback Method
hf	-490.32	kJ/mol	Joback Method
hfus	43.45	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	6.254		Crippen Method
mvol	290.430	ml/mol	McGowan Method
pc	1232.01	kPa	Joback Method
rinpol	2801.00		NIST Webbook
rinpol	2801.00		NIST Webbook
tb	782.41	K	Joback Method
tc	975.05	K	Joback Method
tf	410.01	K	Joback Method
vc	1.121	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.81	J/molxK	782.41	Joback Method
cpg	904.52	J/molxK	814.52	Joback Method
cpg	922.13	J/molxK	846.62	Joback Method
cpg	938.68	J/molxK	878.73	Joback Method
cpg	954.20	J/molxK	910.84	Joback Method
cpg	968.74	J/molxK	942.94	Joback Method
cpg	982.33	J/molxK	975.05	Joback Method
dvisc	0.0014151	Paxs	410.01	Joback Method

dvisc	0.0005902	Paxs	472.08	Joback Method
dvisc	0.0003016	Paxs	534.14	Joback Method
dvisc	0.0001773	Paxs	596.21	Joback Method
dvisc	0.0001152	Paxs	658.28	Joback Method
dvisc	0.0000806	Paxs	720.34	Joback Method
dvisc	0.0000597	Paxs	782.41	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=U415069&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415069&amp;Units=SI</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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