

# 5-Phenylvaleric acid, dodecyl ester

<b>Inchi:</b>	InChI=1S/C23H38O2/c1-2-3-4-5-6-7-8-9-10-16-21-25-23(24)20-15-14-19-22-17-12-11-13
<b>InchiKey:</b>	NRHRKMCJNMJMMM-UHFFFAOYSA-N
<b>Formula:</b>	C23H38O2
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	346.55

## Physical Properties

Property code	Value	Unit	Source
gf	21.27	kJ/mol	Joback Method
hf	-526.32	kJ/mol	Joback Method
hfus	52.15	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.864		Crippen Method
mvol	318.610	ml/mol	McGowan Method
pc	1075.69	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
tb	828.61	K	Joback Method
tc	1021.45	K	Joback Method
tf	447.55	K	Joback Method
vc	1.240	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.10	J/molxK	828.61	Joback Method
cpg	1025.11	J/molxK	860.75	Joback Method
cpg	1042.98	J/molxK	892.89	Joback Method
cpg	1059.76	J/molxK	925.03	Joback Method
cpg	1075.50	J/molxK	957.17	Joback Method
cpg	1090.23	J/molxK	989.31	Joback Method
cpg	1104.00	J/molxK	1021.45	Joback Method
dvisc	0.0009474	Paxs	447.55	Joback Method

dvisc	0.0004261	Paxs	511.06	Joback Method
dvisc	0.0002287	Paxs	574.57	Joback Method
dvisc	0.0001389	Paxs	638.08	Joback Method
dvisc	0.0000923	Paxs	701.59	Joback Method
dvisc	0.0000657	Paxs	765.10	Joback Method
dvisc	0.0000492	Paxs	828.61	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=U406081&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406081&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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