

# Ibuprofen, dodecyl ester

<b>Inchi:</b>	InChI=1S/C25H42O2/c1-5-6-7-8-9-10-11-12-13-14-19-27-25(26)22(4)24-17-15-23(16-18
<b>InchiKey:</b>	AGCFZEYUKWHLRE-UHFFFAOYSA-N
<b>Formula:</b>	C25H42O2
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	374.60

## Physical Properties

Property code	Value	Unit	Source
gf	23.60	kJ/mol	Joback Method
hf	-589.63	kJ/mol	Joback Method
hfus	49.90	kJ/mol	Joback Method
hvap	82.56	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	7.453		Crippen Method
mvol	346.790	ml/mol	McGowan Method
pc	952.60	kPa	Joback Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
tb	878.47	K	Joback Method
tc	1078.84	K	Joback Method
tf	452.61	K	Joback Method
vc	1.339	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.69	J/molxK	878.47	Joback Method
cpg	1150.31	J/molxK	911.86	Joback Method
cpg	1168.66	J/molxK	945.26	Joback Method
cpg	1185.80	J/molxK	978.65	Joback Method
cpg	1201.76	J/molxK	1012.05	Joback Method
cpg	1216.60	J/molxK	1045.44	Joback Method
cpg	1230.37	J/molxK	1078.84	Joback Method
dvisc	0.0008606	Paxs	452.61	Joback Method

dvisc	0.0003410	Paxs	523.59	Joback Method
dvisc	0.0001686	Paxs	594.56	Joback Method
dvisc	0.0000968	Paxs	665.54	Joback Method
dvisc	0.0000619	Paxs	736.52	Joback Method
dvisc	0.0000428	Paxs	807.49	Joback Method
dvisc	0.0000314	Paxs	878.47	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=U390446&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390446&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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