

# Ibuprofen, hexyl ester

<b>Inchi:</b>	InChI=1S/C19H30O2/c1-5-6-7-8-13-21-19(20)16(4)18-11-9-17(10-12-18)14-15(2)3/h9-12
<b>InchiKey:</b>	LLTNCZLHUNOWNU-UHFFFAOYSA-N
<b>Formula:</b>	C19H30O2
<b>SMILES:</b>	CCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	290.44

## Physical Properties

Property code	Value	Unit	Source
gf	-26.92	kJ/mol	Joback Method
hf	-465.79	kJ/mol	Joback Method
hfus	34.36	kJ/mol	Joback Method
hvap	69.21	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.112		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	1557.00		NIST Webbook
rinpol	1557.00		NIST Webbook
tb	741.19	K	Joback Method
tc	938.21	K	Joback Method
tf	384.99	K	Joback Method
vc	1.004	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.82	J/molxK	741.19	Joback Method
cpg	787.26	J/molxK	774.03	Joback Method
cpg	804.63	J/molxK	806.86	Joback Method
cpg	820.94	J/molxK	839.70	Joback Method
cpg	836.24	J/molxK	872.53	Joback Method
cpg	850.55	J/molxK	905.37	Joback Method
cpg	863.91	J/molxK	938.21	Joback Method
dvisc	0.0016841	Paxs	384.99	Joback Method

dvisc	0.0007010	Paxs	444.36	Joback Method
dvisc	0.0003588	Paxs	503.72	Joback Method
dvisc	0.0002115	Paxs	563.09	Joback Method
dvisc	0.0001379	Paxs	622.46	Joback Method
dvisc	0.0000968	Paxs	681.82	Joback Method
dvisc	0.0000720	Paxs	741.19	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U390184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390184&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>mccvol:</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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