

# Ibuprofen, hexadecyl ester

<b>Inchi:</b>	InChI=1S/C29H50O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-31-29(30)26(4)28-21
<b>InchiKey:</b>	ZFCLAIYDFMXKCX-UHFFFAOYSA-N
<b>Formula:</b>	C29H50O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	430.71

## Physical Properties

Property code	Value	Unit	Source
gf	57.28	kJ/mol	Joback Method
hf	-672.19	kJ/mol	Joback Method
hfus	60.26	kJ/mol	Joback Method
hvap	91.47	kJ/mol	Joback Method
log10ws	-9.61		Crippen Method
logp	9.013		Crippen Method
mvol	403.150	ml/mol	McGowan Method
pc	761.42	kPa	Joback Method
rinpol	2147.00		NIST Webbook
rinpol	2147.00		NIST Webbook
tb	969.99	K	Joback Method
tc	1188.47	K	Joback Method
tf	497.69	K	Joback Method
vc	1.563	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1385.13	J/molxK	969.99	Joback Method
cpg	1475.17	J/molxK	1152.06	Joback Method
cpg	1459.93	J/molxK	1115.64	Joback Method
cpg	1443.38	J/molxK	1079.23	Joback Method
cpg	1425.45	J/molxK	1042.82	Joback Method
cpg	1406.06	J/molxK	1006.40	Joback Method
cpg	1489.18	J/molxK	1188.47	Joback Method
dvisc	0.0000172	Paxs	969.99	Joback Method

dvisc	0.0000236	Paxs	891.27	Joback Method
dvisc	0.0000345	Paxs	812.56	Joback Method
dvisc	0.0000545	Paxs	733.84	Joback Method
dvisc	0.0000961	Paxs	655.12	Joback Method
dvisc	0.0001980	Paxs	576.41	Joback Method
dvisc	0.0005126	Paxs	497.69	Joback Method

## Sources

<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=U390450&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390450&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>

## 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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