

Ibuprofen, heptadecyl ester

Inchi:	InChI=1S/C30H52O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-32-30(31)27(4)29
InchiKey:	CZJRTYJMXKJDGM-UHFFFAOYSA-N
Formula:	C30H52O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	444.73

Physical Properties

Property code	Value	Unit	Source
gf	65.70	kJ/mol	Joback Method
hf	-692.83	kJ/mol	Joback Method
hfus	62.85	kJ/mol	Joback Method
hvap	93.69	kJ/mol	Joback Method
log10ws	-10.03		Crippen Method
logp	9.403		Crippen Method
mvol	417.240	ml/mol	McGowan Method
pc	722.63	kPa	Joback Method
rinpol	2262.00		NIST Webbook
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tb	992.87	K	Joback Method
tc	1218.47	K	Joback Method
tf	508.96	K	Joback Method
vc	1.619	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1449.90	J/molxK	992.87	Joback Method
cpg	1471.29	J/molxK	1030.47	Joback Method
cpg	1491.03	J/molxK	1068.07	Joback Method
cpg	1509.24	J/molxK	1105.67	Joback Method
cpg	1525.98	J/molxK	1143.27	Joback Method
cpg	1541.36	J/molxK	1180.87	Joback Method
cpg	1555.46	J/molxK	1218.47	Joback Method
dvisc	0.0004473	Paxs	508.96	Joback Method

dvisc	0.0001718	Paxs	589.61	Joback Method
dvisc	0.0000830	Paxs	670.26	Joback Method
dvisc	0.0000469	Paxs	750.91	Joback Method
dvisc	0.0000296	Paxs	831.57	Joback Method
dvisc	0.0000203	Paxs	912.22	Joback Method
dvisc	0.0000148	Paxs	992.87	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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