

Ibuprofen, nonyl ester

Inchi:	InChI=1S/C22H36O2/c1-5-6-7-8-9-10-11-16-24-22(23)19(4)21-14-12-20(13-15-21)17-18
InchiKey:	OLLWIVFSCIRRQY-UHFFFAOYSA-N
Formula:	C22H36O2
SMILES:	CCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	332.52

Physical Properties

Property code	Value	Unit	Source
gf	-1.66	kJ/mol	Joback Method
hf	-527.71	kJ/mol	Joback Method
hfus	42.13	kJ/mol	Joback Method
hvap	75.88	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	6.282		Crippen Method
mcvol	304.520	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	1715.00		NIST Webbook
tb	809.83	K	Joback Method
tc	1005.55	K	Joback Method
tf	418.80	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.15	J/molxK	809.83	Joback Method
cpg	1029.99	J/molxK	972.93	Joback Method
cpg	1015.38	J/molxK	940.31	Joback Method
cpg	999.73	J/molxK	907.69	Joback Method
cpg	983.00	J/molxK	875.07	Joback Method
cpg	965.15	J/molxK	842.45	Joback Method
cpg	1043.61	J/molxK	1005.55	Joback Method
dvisc	0.0000482	Paxs	809.83	Joback Method
dvisc	0.0000652	Paxs	744.66	Joback Method

dvisc	0.0000937	Paxs	679.49	Joback Method
dvisc	0.0001452	Paxs	614.31	Joback Method
dvisc	0.0002498	Paxs	549.14	Joback Method
dvisc	0.0004974	Paxs	483.97	Joback Method
dvisc	0.0012268	Paxs	418.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U390443&Units=SI

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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