

Ibuprofen, octyl ester

Inchi:	InChI=1S/C21H34O2/c1-5-6-7-8-9-10-15-23-21(22)18(4)20-13-11-19(12-14-20)16-17(2)3
InchiKey:	MKLFYFVVXDTVGT-UHFFFAOYSA-N
Formula:	C21H34O2
SMILES:	CCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	318.49

Physical Properties

Property code	Value	Unit	Source
gf	-10.08	kJ/mol	Joback Method
hf	-507.07	kJ/mol	Joback Method
hfus	39.54	kJ/mol	Joback Method
hvap	73.66	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.892		Crippen Method
mvol	290.430	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinpol	1663.00		NIST Webbook
rinpol	1663.00		NIST Webbook
tb	786.95	K	Joback Method
tc	982.51	K	Joback Method
tf	407.53	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.15	J/molxK	786.95	Joback Method
cpg	904.97	J/molxK	819.54	Joback Method
cpg	922.66	J/molxK	852.14	Joback Method
cpg	939.27	J/molxK	884.73	Joback Method
cpg	954.81	J/molxK	917.33	Joback Method
cpg	969.34	J/molxK	949.92	Joback Method
cpg	982.89	J/molxK	982.51	Joback Method
dvisc	0.0013699	Paxs	407.53	Joback Method

dvisc	0.0005600	Paxs	470.77	Joback Method
dvisc	0.0002830	Paxs	534.00	Joback Method
dvisc	0.0001652	Paxs	597.24	Joback Method
dvisc	0.0001069	Paxs	660.48	Joback Method
dvisc	0.0000747	Paxs	723.71	Joback Method
dvisc	0.0000552	Paxs	786.95	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=U390442&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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