Ibuprofen, ethyl ester

Inchi: InChI=1S/C15H22O2/c1-5-17-15(16)12(4)14-8-6-13(7-9-14)10-11(2)3/h6-9,11-12H,5,10H
InchiKey: HXTFUVWJFLDLJP-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-60.60	kJ/mol	Joback Method
hf	-383.23	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	60.30	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.552		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	1347.00		NIST Webbook
rinpol	1347.00		NIST Webbook
tb	649.67	K	Joback Method
tc	855.34	K	Joback Method
tf	339.91	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.01	J/mol×K	649.67	Joback Method
cpg	564.30	J/mol×K	683.95	Joback Method
cpg	580.59	J/mol×K	718.23	Joback Method
cpg	595.92	J/mol×K	752.51	Joback Method
cpg	610.31	J/mol×K	786.79	Joback Method
cpg	623.79	J/mol×K	821.07	Joback Method
cpg	636.37	J/mol×K	855.34	Joback Method
dvisc	0.0023739	Pa×s	339.91	Joback Method

dvisc	0.0010314	Pa×s	391.54	Joback Method
dvisc	0.0005442	Pa×s	443.16	Joback Method
dvisc	0.0003281	Pa×s	494.79	Joback Method
dvisc	0.0002177	Pa×s	546.42	Joback Method
dvisc	0.0001550	Pa×s	598.04	Joback Method
dvisc	0.0001165	Pa×s	649.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U389552&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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