Ibuprofen, propyl ester

Inchi: InChI=1S/C16H24O2/c1-5-10-18-16(17)13(4)15-8-6-14(7-9-15)11-12(2)3/h6-9,12-13H,5,
InchiKey: QXWDAKBZLIENSO-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: CCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	-52.18	kJ/mol	Joback Method
hf	-403.87	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	62.53	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.942		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1398.00		NIST Webbook
rinpol	1398.00		NIST Webbook
tb	672.55	K	Joback Method
tc	875.45	K	Joback Method
tf	351.18	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.65	J/mol×K	672.55	Joback Method
cpg	679.05	J/mol×K	841.64	Joback Method
cpg	665.29	J/mol×K	807.82	Joback Method
cpg	650.60	J/mol×K	774.00	Joback Method
cpg	634.95	J/mol×K	740.18	Joback Method
cpg	618.31	J/mol×K	706.37	Joback Method
cpg	691.90	J/mol×K	875.45	Joback Method
dvisc	0.0001040	Pa×s	672.55	Joback Method

dvisc	0.0001388	Pa×s	618.99	Joback Method
dvisc	0.0001957	Pa×s	565.43	Joback Method
dvisc	0.0002964	Pa×s	511.87	Joback Method
dvisc	0.0004946	Pa×s	458.30	Joback Method
dvisc	0.0009452	Pa×s	404.74	Joback Method
dvisc	0.0022010	Pa×s	351.18	Joback Method

Sources

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=U389602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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