Ibuprofen, butyl ester

Inchi: InChI=1S/C17H26O2/c1-5-6-11-19-17(18)14(4)16-9-7-15(8-10-16)12-13(2)3/h7-10,13-14
InchiKey: JMYISEMZJYEMCF-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-43.76	kJ/mol	Joback Method
hf	-424.51	kJ/mol	Joback Method
hfus	29.18	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.332		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	1452.00		NIST Webbook
rinpol	1452.00		NIST Webbook
tb	695.43	K	Joback Method
tc	895.94	K	Joback Method
tf	362.45	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.56	J/mol×K	695.43	Joback Method
cpg	735.28	J/mol×K	862.52	Joback Method
cpg	721.30	J/mol×K	829.10	Joback Method
cpg	706.37	J/mol×K	795.68	Joback Method
cpg	690.45	J/mol×K	762.27	Joback Method
cpg	673.53	J/mol×K	728.85	Joback Method
cpg	748.34	J/mol×K	895.94	Joback Method
dvisc	0.0000924	Pa×s	695.43	Joback Method

dvisc	0.0001237	Pa×s	639.93	Joback Method
dvisc	0.0001749	Pa×s	584.44	Joback Method
dvisc	0.0002662	Pa×s	528.94	Joback Method
dvisc	0.0004468	Pa×s	473.44	Joback Method
dvisc	0.0008605	Pa×s	417.95	Joback Method
dvisc	0.0020260	Pa×s	362.45	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=U389604&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