Ibuprofen, isobutyl ester

Inchi: InChI=1S/C17H26O2/c1-12(2)10-15-6-8-16(9-7-15)14(5)17(18)19-11-13(3)4/h6-9,12-14H
InchiKey: IZQZIVHKRMBEMV-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CC(C)COC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-46.20	kJ/mol	Joback Method
hf	-429.79	kJ/mol	Joback Method
hfus	25.66	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.188		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1428.00		NIST Webbook
rinpol	1428.00		NIST Webbook
tb	694.99	K	Joback Method
tc	898.84	K	Joback Method
tf	347.45	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.04	J/mol×K	694.99	Joback Method
cpg	674.33	J/mol×K	728.96	Joback Method
cpg	691.53	J/mol×K	762.94	Joback Method
cpg	707.68	J/mol×K	796.91	Joback Method
cpg	722.81	J/mol×K	830.89	Joback Method
cpg	736.95	J/mol×K	864.86	Joback Method
cpg	750.13	J/mol×K	898.84	Joback Method
dvisc	0.0026098	Pa×s	347.45	Joback Method

dvisc	0.0009827	Pa×s	405.37	Joback Method
dvisc	0.0004724	Pa×s	463.30	Joback Method
dvisc	0.0002672	Pa×s	521.22	Joback Method
dvisc	0.0001694	Pa×s	579.14	Joback Method
dvisc	0.0001167	Pa×s	637.07	Joback Method
dvisc	0.0000855	Pa×s	694.99	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=U389599&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

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