Flurbiprofen, hydroxy, bis-methylated

Inchi: InChI=1S/C17H17FO3/c1-11(17(19)21-3)13-6-9-15(16(18)10-13)12-4-7-14(20-2)8-5-12/h
InchiKey: KETBZMOPTVEHCA-UHFFFAOYSA-N
Formula: C17H17FO3
SMILES: COC(=O)C(C)c1ccc(-c2ccc(OC)cc2)c(F)c1
Mol. weight [g/mol]: 288.31

Physical Properties

Property code	Value	Unit	Source
gf	-247.98	kJ/mol	Joback Method
hf	-533.97	kJ/mol	Joback Method
hfus	30.23	kJ/mol	Joback Method
hvap	70.34	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.778		Crippen Method
mcvol	217.950	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	754.20	K	Joback Method
tc	977.22	K	Joback Method
tf	451.73	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.77	J/mol×K	754.20	Joback Method
cpg	619.86	J/mol×K	791.37	Joback Method
cpg	633.81	J/mol×K	828.54	Joback Method
cpg	646.63	J/mol×K	865.71	Joback Method
cpg	658.34	J/mol×K	902.88	Joback Method
cpg	668.96	J/mol×K	940.05	Joback Method
cpg	678.51	J/mol×K	977.22	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=R201635&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
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