Ibuprofen methyl ester

Other names:	Benzeneacetic acid, «alpha»-methyl-4-(2-methylpropyl)-, methyl ester
	Methyl ester of Ibuprofen
	Ibuprofen methyl deriv
	Ibuprofen methyl derivative
	Methyl 2-(4-isobutylphenyl)propanoate
	Motrin methyl ester
	Racemic ibuprofen methyl ester
	Methyl 2-(4'-isobutylphenyl)propanoate
	2-(4-Isobutylphenyl)propionic acid methyl ester
	methyl 2-(4-isopropylphenyl)propionate
	Ibuprofen Me
Inchi:	InChI=1S/C14H20O2/c1-10(2)9-12-5-7-13(8-6-12)11(3)14(15)16-4/h5-8,10-11H,9H2,1-4
InchiKey:	YNZYUHPFNYBBFF-UHFFFAOYSA-N
Formula:	C14H20O2
SMILES:	COC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	220.31
CAS:	61566-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-69.02	kJ/mol	Joback Method
hf	-362.59	kJ/mol	Joback Method
hfus	21.41	kJ/mol	Joback Method
hvap	58.08	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.162		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook
tb	626.79	K	Joback Method
tc	835.57	K	Joback Method
tf	328.64	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.71	J/mol×K	626.79	Joback Method
cpg	511.55	J/mol×K	661.59	Joback Method
cpg	527.43	J/mol×K	696.38	Joback Method
cpg	542.37	J/mol×K	731.18	Joback Method
cpg	556.40	J/mol×K	765.97	Joback Method
cpg	569.53	J/mol×K	800.77	Joback Method
cpg	581.79	J/mol×K	835.57	Joback Method
dvisc	0.0025399	Pa×s	328.64	Joback Method
dvisc	0.0011173	Pa×s	378.33	Joback Method
dvisc	0.0005947	Pa×s	428.02	Joback Method
dvisc	0.0003610	Pa×s	477.72	Joback Method
dvisc	0.0002407	Pa×s	527.41	Joback Method
dvisc	0.0001721	Pa×s	577.10	Joback Method
dvisc	0.0001298	Pa×s	626.79	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61566345&Units=SI
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

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