Flurbiprofen

Other names:	(.+/-.)-2-(2-Fluoro-4-biphenylyl)propionic acid
	(.+/-.)-2-Fluoro-«alpha»-methyl-4-biphenylacetic acid
	(.+/-.)-2-Fluoro-Â«alphaÂ»-methyl-4-biphenylacetic acid
	(.+/-.)-Flurbiprofen
	2-(2-Fluoro-4-biphenylyl)propionic acid
	2-(2-fluoro-4-biphenyl)propionic acid
	2-(2-fluoro-4-biphenylyl)propanoic acid
	2-Fluoro-«alpha»-methyl(1,1'-biphenyl)-4-acetic acid
	2-Fluoro-«alpha»-methyl-4-biphenylacetic acid
	2-Fluoro-«alpha»-methyl[1,1'-biphenyl]-4-acetic acid (flurbiprofen)
	2-Fluoro-Â«alphaÂ»-methyl(1,1'-biphenyl)-4-acetic acid
	2-Fluoro-Â«alphaÂ»-methyl-4-biphenylacetic acid
	2-Fluoro-Â«alphaÂ»-methyl[1,1'-biphenyl]-4-acetic acid (flurbiprofen)
	3-Fluoro-4-phenylhydratropic acid
	4-Biphenylacetic acid, 2-fluoro-«alpha»-methyl-
	4-Biphenylacetic acid, 2-fluoro-Â«alphaÂ»-methyl-
	4-biphenylacetic acid, 2-fluoro-.alpha.-methyl-
	Adfeed
	Ansaid
	Antadys
	BTS 18322
	Cebutid
	FP 70
	Flurofen
	Froben
	Stayban
	U-27182
	Zepolas
	[1,1'-Biphenyl]-4-acetic acid, 2-fluoro-«alpha»-methyl-
	[1,1'-Biphenyl]-4-acetic acid, 2-fluoro-«alpha»-methyl-, (.+/-.)-
	[1,1'-Biphenyl]-4-acetic acid, 2-fluoro-Â«alphaÂ»-methyl-
	[1,1'-Biphenyl]-4-acetic acid, 2-fluoro-Â«alphaÂ»-methyl-, (.+/-.)-
	[1,1'-biphenyl]-4-acetic acid, 2-fluoro-.alpha.-methyl-
	dl-Flurbiprofen
	hydratropic acid, 3-fluoro-4-phenyl-
Inchi:	InChI=1S/C15H13FO2/c1-10(15(17)18)12-7-8-13(14(16)9-12)11-5-3-2-4-6-11/h2-10H,1H
InchiKey:	SYTBZMRGLBWNTM-UHFFFAOYSA-N
Formula:	C15H13FO2
SMILES:	CC(C(=O)O)c1ccc(-c2ccccc2)c(F)c1
Mol. weight [g/mol]:	244.26

CAS: 5104-49-4

Physical Properties

Property code	Value	Unit	Source
gf	-182.01	kJ/mol	Joback Method
hf	-369.01	kJ/mol	Joback Method
hfus	27.15	kJ/mol	Joback Method
hvap	77.08	kJ/mol	Joback Method
log10ws	-3.65		Aqueous Solubility Prediction Method
logp	3.681		Crippen Method
mcvol	183.900	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	750.80	K	Joback Method
tc	969.56	K	Joback Method
tf	384.27	K	Aqueous Solubility Prediction Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.23	J/mol×K	933.10	Joback Method
cpg	499.82	J/mol×K	750.80	Joback Method
cpg	511.81	J/mol×K	787.26	Joback Method
cpg	522.89	J/mol×K	823.72	Joback Method
cpg	533.12	J/mol×K	860.18	Joback Method
cpg	542.55	J/mol×K	896.64	Joback Method
cpg	559.20	J/mol×K	969.56	Joback Method
hfust	27.90	kJ/mol	386.70	NIST Webbook
hsubt	108.40 ± 0.50	kJ/mol	354.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5104494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Flurbiprofen in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je034099b
Solubility of Flurbiprofen in CO2 and CO2 + Methanol:	https://www.doi.org/10.1021/je900674t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume