Ibuprofen

Other names:

(.+/-.)-2-(p-Isobutylphenyl)propionic acid
(.+/-.)-p-Isobutylhydratropic acid
(2S)-2-[4-(2-methylpropyl)phenyl]propanoic acid
(RS)-Ibuprofen
(S)-2-(4-isobutylphenyl)propanoic acid
(±) «alpha»-methyl-4-(isobutyl)phenylacetic acid (ibuprofen)
(Â±) Â«alphaÂ»-methyl-4-(isobutyl)phenylacetic acid (ibuprofen)
2-(4-Isobutylphenyl)propanoic acid
2-(p-Isobutylphenyl)propionic acid
4-Isobutyl-«alpha»-methylphenylacetic acid
4-Isobutyl-Â«alphaÂ»-methylphenylacetic acid
4-Isobutylhydratropic acid
4-Isobutylphenyl)-«alpha»-methylacetic acid
4-Isobutylphenyl)-Â«alphaÂ»-methylacetic acid
Acide (isobutyl-4 phenyl)-2 propionique
Adran
Advil
Andran
Anflagen
Apsifen
Artril 300
Benzeneacetic acid, «alpha»-methyl-4-(2-methylpropyl), (.+/-.)-
Benzeneacetic acid, «alpha»-methyl-4-(2-methylpropyl)-
Benzeneacetic acid, Â«alphaÂ»-methyl-4-(2-methylpropyl), (.+/-.)-
Benzeneacetic acid, Â«alphaÂ»-methyl-4-(2-methylpropyl)-
Bluton
Brufanic
Brufen
Buburone
Burana
Butacortelone
Butylenin
Carol
Cobo
Dibufen
Dolgin
Dolgit
Ebufac
Emodin
Epobron

Haltran
Hydratropic acid, p-isobutyl-
IP-82
Ibu-slo
Ibufen
Ibupril
Ibuprocin
Lamidon
Liptan
Medipren
Midol 200
Motrin
Mynosedin
Napacetin
Nobfelon
Nobfen
Nobgen
Nuprin
Nurofen
Optifen
Ostofen
Panafen
Pantrop
PediaProfen
Proartinal
Proflex
Propanoic acid, 2-(4-isobutylphenyl)
Quadrax
R.D. 13621
RD 13621
Rebugen
Roidenin
S-(+)-ibuprofen
S-ibuprofen
Trendar
U-18,573
Uprofen
dexibuprofen
p-Isobutyl-2-phenylpropionic acid
p-Isobutylhydratropic acid
«alpha»-(4-Isobutylphenyl)propionic acid
«alpha»-(p-isobutylphenyl)propionic acid
«alpha»-2-(p-Isobutylphenyl)propionic acid

	«alpha»-Methyl-4-(2-methylpropyl)benzeneacetic acid
	Â«alphaÂ»-(4-Isobutylphenyl)propionic acid
	Â«alphaÂ»-(p-isobutylphenyl)propionic acid
	Â«alphaÂ»-2-(p-Isobutylphenyl)propionic acid
	Â«alphaÂ»-Methyl-4-(2-methylpropyl)benzeneacetic acid
Inchi:	InChI=1S/C13H18O2/c1-9(2)8-11-4-6-12(7-5-11)10(3)13(14)15/h4-7,9-10H,8H2,1-3H3,(H
InchiKey:	HEFNNWSXXWATRW-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CC(C)Cc1ccc(C(C)C(=O)O)cc1
Mol. weight [g/mol]:	206.28
CAS:	15687-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-109.26	kJ/mol	Joback Method
hf	-361.96	kJ/mol	Joback Method
hfus	21.72	kJ/mol	Joback Method
hvap	70.12	kJ/mol	Joback Method
log10ws	-3.34		Aqueous Solubility Prediction Method
logp	3.073		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1594.00		NIST Webbook
rinpol	1630.20		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	673.67	K	Joback Method
tc	874.24	K	Joback Method
tf	348.20	K	Solid-state interaction of ibuprofen and Neusilin US2
tf	347.65	K	Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide

tf	349.20	K	Measurement and Correlation of the Solid-Liquid-Gas Equilibria for the Carbon Dioxide + S-(+)-Ibuprofen and Carbon Dioxide + RS-(+/-)-Ibuprofen Systems
tf	347.70	K	Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid
tf	347.70	K	Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds
tf	420.31	K	Aqueous Solubility Prediction Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.24	J/mol×K	740.53	Joback Method
cpg	545.74	J/mol×K	874.24	Joback Method
cpg	535.91	J/mol×K	840.81	Joback Method
cpg	525.41	J/mol×K	807.38	Joback Method
cpg	514.19	J/mol×K	773.95	Joback Method
cpg	475.97	J/mol×K	673.67	Joback Method
cpg	489.51	J/mol×K	707.10	Joback Method
dvisc	0.0014382	Pa×s	408.91	Joback Method
dvisc	0.0005304	Pa×s	461.86	Joback Method
dvisc	0.0002401	Pa×s	514.82	Joback Method
dvisc	0.0001260	Pa×s	567.77	Joback Method
dvisc	0.0000738	Pa×s	620.72	Joback Method
dvisc	0.0052478	Pa×s	355.96	Joback Method
dvisc	0.0000471	Pa×s	673.67	Joback Method
hfust	25.70	kJ/mol	350.90	NIST Webbook
hfust	26.65	kJ/mol	348.00	NIST Webbook
hfust	26.60	kJ/mol	346.40	NIST Webbook
hfust	27.94	kJ/mol	347.60	NIST Webbook
hfust	39.50	kJ/mol	350.40	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solubilities of Ibuprofen in Different Pure Solvents:	https://www.doi.org/10.1021/je100255z
Effect of Solvent Composition and Temperature on the Solubility of Ibuprofen in Aqueous Ethanol:	https://www.doi.org/10.1021/je400819z
Thermodynamic study of the solubility of ibuprofen and naproxen in some ethanol + propylene glycol mixtures:	https://www.doi.org/10.1016/j.fluid.2007.07.076
Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquids:	https://www.doi.org/10.1016/j.fluid.2015.03.053
Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je049551l
Solid−Liquid Phase Equilibrium and Ternary Phase Diagrams of Ibuprofen Nicotinamide Cocrystals in Ethanol and Ethanol/Water Mixtures at (298.15 and 313.15) K:	https://www.doi.org/10.1021/je5011455
Phase Equilibria of the System Drug + Water:	https://www.doi.org/10.1021/je101163y
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of Pharmaceutical Compounds in Ionic Liquids :	https://www.doi.org/10.1021/je101040p
Solubility of Dexibuprofen in Different Solvents from (263.15 to 293.15) K:	https://www.doi.org/10.1021/je101165m
Measurement and Correlation of the Solid-Liquid-Gas Equilibria for the Carbon Dioxide + S-(+) Ibuprofen and Carbon Dioxide + Rac-(±) Ibuprofen Systems:	https://www.doi.org/10.1021/je034228o
Measurement and Correlation for Solubility of Dexibuprofen in Different Solvents from (263.15 to 293.15) K:	https://www.doi.org/10.1016/j.tca.2012.04.016
Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds:	https://www.doi.org/10.1016/j.fluid.2014.10.033
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15687271&Units=SI
Solid-state interaction of ibuprofen and Neusilin US2:	https://www.doi.org/10.1016/j.tca.2010.05.009

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
hfust:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume