Ketoprofen

Other names:
(+)«alpha»-(3-benzoylphenyl)propionic acid ((+)-ketoprofen)
(+)Â«alphaÂ»-(3-benzoylphenyl)propionic acid ((+)-ketoprofen)
(.+/-.)-3-Benzoyl-«alpha»-methylbenzeneacetic acid
(.+/-.)-3-Benzoyl-Â«alphaÂ»-methylbenzeneacetic acid
(.+/-.)-m-Benzoylhydratropic acid
19583 RP
2-(3-Benzoylphenyl)propionic acid
2-(m-Benzoylphenyl)propionic acid
3-Benzoyl-«alpha»-methylbenzeneacetic acid
3-Benzoyl-Â«alphaÂ»-methylbenzeneacetic acid
3-Benzoylhydratropic acid
Alrheumat
Alrheumun
Aneol
Benzeneacetic acid, 3-benzoyl-«alpha»-methyl-
Benzeneacetic acid, 3-benzoyl-Â«alphaÂ»-methyl-
Capisten
Dexal
Epatec
Fastum
Iso-K
Kefenid
Ketoprofene
Ketopron
Lertus
Menamin
Meprofen
Orudis
Orugesic
Oruvail
Oscorel
Profenid
Propionic acid, 2-(3-benzoylphenyl)-
RP-19583
RU 4733
Racemic ketoprofen
Toprec
Toprek
m-Benzoylhydratropic acid

Inchi:
InChI=1S/C16H14O3/c1-11(16(18)19)13-8-5-9-14(10-13)15(17)12-6-3-2-4-7-12/h2-11H,1

InchiKey: DKYWVDODHFEZIM-UHFFFAOYSA-N
Formula: C16H14O3
SMILES: CC(C(=O)O)c1cccc(C(=O)c2ccccc2)c1
Mol. weight [g/mol]: 254.28
CAS: 22071-15-4

Physical Properties

Property code	Value	Unit	Source
gf	-98.07	kJ/mol	Joback Method
hf	-294.65	kJ/mol	Joback Method
hfus	28.65	kJ/mol	Joback Method
hvap	86.21	kJ/mol	Joback Method
log10ws	-3.45		Aqueous Solubility Prediction Method
log10ws	-3.21		Aqueous Solubility Prediction Method
logp	3.106		Crippen Method
mcvol	197.790	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	2185.00		NIST Webbook
tb	823.30	K	Joback Method
tc	1052.13	K	Joback Method
tf	367.12	K	Aqueous Solubility Prediction Method
tf	367.01	K	Aqueous Solubility Prediction Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.11	J/mol×K	823.30	Joback Method
cpg	568.42	J/mol×K	861.44	Joback Method
cpg	578.78	J/mol×K	899.58	Joback Method
cpg	588.24	J/mol×K	937.72	Joback Method
cpg	596.87	J/mol×K	975.85	Joback Method
cpg	604.74	J/mol×K	1013.99	Joback Method
cpg	611.91	J/mol×K	1052.13	Joback Method

dvisc	0.0001707	Pa×s	595.18	Joback Method
dvisc	0.0003532	Pa×s	538.15	Joback Method
dvisc	0.0008679	Pa×s	481.12	Joback Method
dvisc	0.0000937	Pa×s	652.21	Joback Method
dvisc	0.0000567	Pa×s	709.24	Joback Method
dvisc	0.0000369	Pa×s	766.27	Joback Method
dvisc	0.0000255	Pa×s	823.30	Joback Method
hfust	37.30	kJ/mol	368.00	NIST Webbook
hfust	25.04	kJ/mol	369.00	NIST Webbook
hfust	28.23	kJ/mol	367.40	NIST Webbook
hsubt	110.10 ± 0.50	kJ/mol	353.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Thermodynamic analysis of the solubility of ketoprofen in some propylene glycol + water cosolvent mixtures:	https://www.doi.org/10.1016/j.fluid.2010.03.031
Solution Thermodynamics of Ketoprofen in Ethanol + Water Cosolvent Mixtures:	https://www.doi.org/10.1021/je9002866
Cosolubility of Benzocaine, Lidocaine, and Procaine in Liquid and Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je034163p
Solubility and Association of Ketoprofen and Aspirin in Supercritical CO2 by Infrared Spectroscopy:	https://www.doi.org/10.1021/acs.jced.5b00812
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22071154&Units=SI

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