Indomethacin

Other names:

(1-p-Chlorobenzoyl-5-methoxy-2-methylindol-3-yl)acetic acid
1-(4-Chlorobenzoyl)-2-methyl-5-methoxyindole-3-acetic acid
1-(4-Chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-acetic acid (indomethacin)
1-(4-Chlorobenzoyl)-5-methoxy-2-methylindole-3-acetic acid
1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-3-acetic acid
1-(p-Chlorobenzoyl)-2-methyl-5-methoxy-3-indole-acetic acid
1-(p-Chlorobenzoyl)-2-methyl-5-methoxyindole-3-acetic acid
1-(p-Chlorobenzoyl)-5-methoxy-2-methyl-3-indolylacetic acid
1-(p-Chlorobenzoyl)-5-methoxy-2-methylindol-3-acetic acid
1-(p-Chlorobenzoyl)-5-methoxy-2-methylindole-3-acetic acid
1-p-Cloro-benzoil-5-metoxi-2-metilindol-3-acido acetico
1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-
2-[1-(4-chlorobenzoyl)-5-methoxy-2-methylindol-3-yl]acetic acid
Amuno
Argun
Artracin
Artrinovo
Artrivia
Bonidin
Catlep
Chibro-amuno
Chrono-indicid
Confortid
Dolcidium
Dolovin
Durametacin
Elmetacin
Idomethine
Imbrilon
Inacid
Indacin
Indo-Rectolmin
Indo-phlogont
Indo-tablinen
Indocid
Indocin
Indocollyre
Indole-3-acetic acid, 1-(p-chlorobenzoyl)-5-methoxy-2-methyl-
Indomecol
Indomed

Indomee
Indometacin
Indometacine
Indometacyna
Indomethacine
Indomethazine
Indomethine
Indometicina
Indomod
Indonol
Indoptic
Indoptol
Indorektal
Indoxen
Inflazon
Infrocin
Innamit
Inteban
Inteban sp
Kwas 1-(p-chlorobenzoilo)-2-metylo-5-metoksy-3-indolilooctowy
Lausit
Metacen
Metartril
Methazine
Metindol
Mezolin
Miametan
Mikametan
Mobilan
N-(p-Chlorobenzoyl)-2-methyl-5-methoxy-3-indolylacetic acid
N-p-Chlorbenzoyl-5-methoxy-2-methylindole-3-acetic acid
NCI-C56144
Reumacide
Rheumacin LA
Sadoreum
Tannex
Vonum
«alpha»-(1-(p-Chlorobenzoyl)-2-methyl-5-methoxy-3-indolyl)acetic acid
Â«alphaÂ»-(1-(p-Chlorobenzoyl)-2-methyl-5-methoxy-3-indolyl)acetic acid

Inchi: InChI=1S/C19H16ClNO4/c1-11-15(10-18(22)23)16-9-14(25-2)7-8-17(16)21(11)19(24)12-

InchiKey: CGIGDMFJXJATDK-UHFFFAOYSA-N

Formula: C19H16ClNO4

SMILES: COc1ccc2c(c1)c(CC(=O)O)c(C)n2C(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 357.79
CAS: 53-86-1

Physical Properties

Property code	Value	Unit	Source
hfus	55.10	kJ/mol	Thermodynamic analysis and enthalpy-entropy compensation for the solubility of indomethacin in aqueous and non-aqueous mixtures
log10ws	-4.69		Aqueous Solubility Prediction Method
log10ws	-2.94		Aqueous Solubility Prediction Method
logp	3.927		Crippen Method
mcvol	252.990	ml/mol	McGowan Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
rinpol	2685.00		NIST Webbook
tf	432.10	K	Aqueous Solubility Prediction Method
tf	432.10	K	Aqueous Solubility Prediction Method
tf	433.60	K	Solubility of pharmaceuticals in water and alcohols
tf	433.10	K	(Solid + liquid) phase diagram for (indomethacin + nicotinamide)- methanol or methanol/ethyl acetate mixture and solubility behavior of 1:1 (indomethacin + nicotinamide) co-crystal at T = (298.15 and 313.15) K
tf	433.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	43.50	kJ/mol	434.50	NIST Webbook
hfust	36.50	kJ/mol	435.20	NIST Webbook

hfust	39.99	kJ/mol	434.00	NIST Webbook
hfust	37.90	kJ/mol	433.00	NIST Webbook
hfust	37.80	kJ/mol	433.00	NIST Webbook
hfust	36.49	kJ/mol	435.20	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53861&Units=SI
Solubilities of Organic Semiconductors and Nonsteroidal Anti-inflammatory Drugs in Pure and Mixed Organic Solvents: Measurement and Modeling with Hansen Solubility Parameter:	https://www.doi.org/10.1021/acs.jced.8b00536
(Solid + liquid) phase diagram for (indomethacin + nicotinamide)-methanol or methanol/ethyl acetate mixture and solubility behavior of 1:1 (indomethacin + nicotinamide) co-crystal at T = (298.15 and 313.15) K:	https://www.doi.org/10.1016/j.jct.2015.01.015
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility and preferential solvation of indomethacin in 1,4-dioxane + water solvent mixtures:	https://www.doi.org/10.1016/j.fluid.2010.09.027
Thermodynamic analysis and enthalpy-entropy compensation for the solubility of indomethacin in aqueous and non-aqueous mixtures:	https://www.doi.org/10.1016/j.fluid.2011.06.016
Solution thermodynamics of indomethacin in propylene glycol + water mixtures:	https://www.doi.org/10.1016/j.fluid.2011.11.001
Solubility of pharmaceuticals in water and alcohols:	https://www.doi.org/10.1016/j.fluid.2015.02.018
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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