Sulindac

Other names:

((1Z)-5-Fluoro-2-methyl-1-[4-(methylsulfinyl)benzylidene]-1H-inden-3-yl)acetic acid
(Z)-2-(5-fluoro-2-methyl-1-(4-(methylsulfinyl)benzylidene)-1H-inden-3-yl)acetic acid
(Z)-5-Fluoro-2-methyl-1-((p-(methylsulfinyl)phenyl)methylene)-1H-indene-3-acetic acid
(Z)-5-fluoro-2-methyl-1-[p-(methylsulfinyl)benzylidene]indene-3-acetic acid
(Z)-5-fluoro-2-methyl-1-[p-(methylsulfinyl)benzylidene]indene-3-acetic acid (sulindac)
1H-Indene-3-acetic acid, 5-fluoro-2-methyl-1-[[4-(methylsulfinyl)phenyl]methylene]-, (Z)-
Aflodac
Algocetil
Arthrocine
Artribid
Citireuma
Clinoril
Clisundac
Imbaral
MK 231
Mobilin
Reumofil
Reumyl
Sudac
Sulindac sulfoxide
Sulinol
Sulreuma
cis-5-Fluoro-2-methyl-1-((4-(methylsulfinyl)phenyl)methylene)-1H-indene-3-acetic acid
cis-5-Fluoro-2-methyl-1-[(p-methylsulfinyl)benzylidene]indene-3-acetic acid

Inchi: InChI=1S/C20H17FO3S/c1-12-17(9-13-3-6-15(7-4-13)25(2)24)16-8-5-14(21)10-19(16)18

InchiKey: MLKXDPUZXIRXEP-RQZCQDPDSA-N

Formula: C20H17FO3S

SMILES: CC1=C(CC(=O)O)c2cc(F)ccc2C1=Cc1ccc(S(C)=O)cc1

Mol. weight [g/mol]: 356.41

CAS: 38194-50-2

Physical Properties

Property code	Value	Unit	Source
gf	-240.19	kJ/mol	Joback Method
hf	-480.13	kJ/mol	Joback Method
hfus	48.82	kJ/mol	Joback Method

hvap	104.61	kJ/mol	Joback Method
log10ws	-3.68		Aqueous Solubility Prediction Method
logp	4.366		Crippen Method
mcvol	257.110	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
tb	956.07	K	Joback Method
tc	1185.39	K	Joback Method
tf	458.15	K	Thermal characterization of some polymorph solvates of the anti-inflammatory/anti-cancer sulindac
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.14	J/mol×K	1147.17	Joback Method
cpg	757.03	J/mol×K	956.07	Joback Method
cpg	767.82	J/mol×K	994.29	Joback Method
cpg	777.84	J/mol×K	1032.51	Joback Method
cpg	787.18	J/mol×K	1070.73	Joback Method
cpg	795.92	J/mol×K	1108.95	Joback Method
cpg	811.93	J/mol×K	1185.39	Joback Method
hfust	33.40	kJ/mol	460.20	NIST Webbook

Sources

Thermal characterization of some polymorph solvates of the anti-inflammatory/anti-cancer sulindac: https://www.doi.org/10.1016/j.tca.2016.01.006

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38194502&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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