Diflunisal

Other names:	2',4'-Difluoro-4-hydroxy-(1',1-diphenyl)-3-carboxylic acid
	2',4'-Difluoro-4-hydroxy-(1,1'-biphenyl)-3-carboxylic acid
	2',4'-Difluoro-4-hydroxy-3-biphenylcarboxylic acid
	2-(Hydroxy)-5-(2,4-difluorophenyl)benzoic acid
	3-Biphenylcarboxylic acid, 2',4'-difluoro-4-hydroxy-
	5-(2,4-Difluorophenyl)salicylic acid
	5-[2,4-Difluorophenyl]salicylic acid (diflunisal)
	Adomal
	Difludol
	Diflusinal
	Dolisal
	Dolobid
	Dolobil
	Dolobis
	Flovacil
	Fluniget
	Fluodonil
	Flustar
	MK 647
	[1,1'-Biphenyl]-3-carboxylic acid, 2',4'-difluoro-4-hydroxy-
Inchi:	InChI=1S/C13H8F2O3/c14-8-2-3-9(11(15)6-8)7-1-4-12(16)10(5-7)13(17)18/h1-6,16H,(H,
InchiKey:	HUPFGZXOMWLGNK-UHFFFAOYSA-N
Formula:	C13H8F2O3
SMILES:	O=C(O)c1cc(-c2ccc(F)cc2F)ccc1O
Mol. weight [g/mol]:	250.20
CAS:	22494-42-4

Physical Properties

Property code	Value	Unit	Source
gf	-555.47	kJ/mol	Joback Method
hf	-707.34	kJ/mol	Joback Method
hfus	33.97	kJ/mol	Joback Method
hvap	85.88	kJ/mol	Joback Method
log10ws	-5.94		Aqueous Solubility Prediction Method
log10ws	-4.11		Aqueous Solubility Prediction Method

log10ws	-4.48		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	3.036		Crippen Method
mcvol	163.360	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	2031.00		NIST Webbook
rinpol	2031.00		NIST Webbook
tb	790.35	K	Joback Method
tc	1011.96	K	Joback Method
tf	486.65	K	Aqueous Solubility Prediction Method
tf	486.65	K	Aqueous Solubility Prediction Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.53	J/mol×K	790.35	Joback Method
cpg	452.35	J/mol×K	827.28	Joback Method
cpg	460.66	J/mol×K	864.22	Joback Method
cpg	468.54	J/mol×K	901.15	Joback Method
cpg	476.06	J/mol×K	938.09	Joback Method
cpg	483.30	J/mol×K	975.02	Joback Method
cpg	490.36	J/mol×K	1011.96	Joback Method
hsubt	119.30 ± 0.60	kJ/mol	381.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22494424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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
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