Felodipine

Other names:

(.+/-.) Ethyl methyl 4-(2,3-dichlorophenyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate

(.+/-.)-Felodipine

(±) Ethyl methyl 1,4-dihydro-2,6-dimethyl-4-(2,3-dichlorophenyl)-3,5-pyridine dicarboxylate (felodipine)

(A±) Ethyl methyl 1,4-dihydro-2,6-dimethyl-4-(2,3-dichlorophenyl)-3,5-pyridine dicarboxylate (felodipine)

3,5-Pyridinedicarboxylic acid, 4-(2,3-dichlorophenyl)-1,4-dihydro-2,6-dimethyl-, ethyl methyl ester

3-Ethyl 5-methyl 4-(2,3-dichlorophenyl)-2,6-dimethyl-1,4-dihydro-3,5-pyridinedicarboxylate

4-(2,3-Dichlorophenyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinecarboxylic acid ethyl methyl ester

Agon

Ethyl methyl 4-(2,3-dichlorophenyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate

Feloday

Felodipine (dl form)

Flodil

H-154/82

Hydac

Munobal

O3-ethyl O5-methyl 4-(2,3-dichlorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate

Plandil

Plendil

Prevex

Splendil

dl-Felodipine

Inchi: InChI=1S/C18H19Cl2NO4/c1-5-25-18(23)14-10(3)21-9(2)13(17(22)24-4)15(14)11-7-6-8-

InchiKey: RZTAMFZIAATZDJ-UHFFFAOYSA-N

Formula: C18H19Cl2NO4

SMILES: CCOC(=O)C1=C(C)NC(C)=C(C(=O)OC)C1c1cccc(Cl)c1Cl

Mol. weight [g/mol]: 384.25

CAS: 72509-76-3

Physical Properties

Property code	Value	Unit	Source
gf	-164.31	kJ/mol	Joback Method
hf	-560.53	kJ/mol	Joback Method
hfus	51.92	kJ/mol	Joback Method
hvap	96.76	kJ/mol	Joback Method
log10ws	-5.68		Aqueous Solubility Prediction Method
logp	3.964		Crippen Method

mcvol	270.600	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2718.20		NIST Webbook
rinpol	2718.20		NIST Webbook
tb	961.66	K	Joback Method
tc	1200.94	K	Joback Method
tf	712.25	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.23	J/mol×K	961.66	Joback Method
cpg	796.85	J/mol×K	1001.54	Joback Method
cpg	805.89	J/mol×K	1041.42	Joback Method
cpg	813.32	J/mol×K	1081.30	Joback Method
cpg	819.14	J/mol×K	1121.18	Joback Method
cpg	823.33	J/mol×K	1161.06	Joback Method
cpg	825.86	J/mol×K	1200.94	Joback Method
hfust	34.80	kJ/mol	412.30	NIST Webbook
hfust	35.21	kJ/mol	414.90	NIST Webbook

Sources

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=C72509763&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Felodipine and Nitrendipine in Liquid and Supercritical Carbon Dioxide: by Cloud Point and UV Spectroscopy:	https://www.doi.org/10.1021/je0603729
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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