Nifedipine

Other names:	3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-, dimethyl ester 4-(2-Nitrophenyl)-2,6-dimethyl-3,5-dicarbomethoxy-1,4-dihydropyridine Adalat Adalat CC Bay a 1040 Citilat Cordipin Dimethyl 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-3,5-pyridinedicarboxylate Dimethyl 1,4-dihydro-2,6-dimethyl-4-(o-nitrophenyl)-3,5-pyridinedicarboxylate Dimethyl 4-(2-nitrophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate Fenihidine Hexadilat Introcar Kordafen Nifedicor Nifedin Nifelan Nifelat Nifensar XL Orix Oxcord Pidilat Procardia Procardia XL Sepamit Tibricol Zenusin dimethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate
Inchi:	InChI=1S/C17H18N2O6/c1-9-13(16(20)24-3)15(14(10(2)18-9)17(21)25-4)11-7-5-6-8-12(
InchiKey:	HYIMSNHJOBLJNT-UHFFFAOYSA-N
Formula:	C17H18N2O6
SMILES:	COC(=O)C1=C(C)NC(C)=C(C(=O)OC)C1c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	346.33
CAS:	21829-25-4

Physical Properties

Property code	Value	Unit	Source

gf	-103.69	kJ/mol	Joback Method
hf	-507.70	kJ/mol	Joback Method
hfus	52.69	kJ/mol	Joback Method
hvap	101.70	kJ/mol	Joback Method
log10ws	-4.64		Aqueous Solubility Prediction Method
log10ws	-4.76		Estimated Solubility Method
logp	2.176		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2536.74		NIST Webbook
rinpol	2536.74		NIST Webbook
tb	1010.78	K	Joback Method
tc	1263.21	K	Joback Method
tf	446.65	K	Determination and correlation thermodynamic models for solid liquid equilibrium of the Nifedipine in pure and mixture organic solvents
tt	317.60	K	Endothermic features on heating of glasses show that the second glass to liquid transition of water was phenomenologically-mistaken
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.16	J/mol×K	1010.78	Joback Method
cpg	789.00	J/mol×K	1052.85	Joback Method
cpg	796.04	J/mol×K	1094.92	Joback Method
cpg	801.27	J/mol×K	1137.00	Joback Method
cpg	804.67	J/mol×K	1179.07	Joback Method
cpg	806.24	J/mol×K	1221.14	Joback Method
cpg	805.95	J/mol×K	1263.21	Joback Method

Sources

Determining the Solubility of Nifedipine and Quinine in Supercritical Fluid Carbon Dioxide Using Continuously Stirred Static Solubility Apparatus Interfaced with Online Supercritical Fluid Chromatography:	https://www.doi.org/10.1021/acs.jced.7b00012
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Endothermic features on heating of glasses show that the second glass to liquid transition of water was phenomenologically mistaken:	https://www.doi.org/10.1016/j.tca.2016.11.011
Determination and correlation thermodynamic models for solid liquid equilibrium of the Nifedipine in pure and mixed organic solvents:	https://www.doi.org/10.1016/j.jct.2016.07.035
Phase solubility studies of poorly soluble drug molecules by using O-phosphorylated calixarenes as drug solubilizing agents:	https://www.doi.org/10.1021/je200992c
Orrmen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21829254&Units=SI

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
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
tt:	Triple Point Temperature
vc:	Critical Volume