Nitrendipine

Other names:	(.+/-.)-Ethyl methyl 1,4-dihydro-2,6-dimethyl-4-(m-nitrophenyl)-3,5-pyridinedicarboxylate (.+/-.)-Nitrendipine 1,4-Dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylic acid ethyl methyl ester 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, 3-ethyl 5-methyl ester 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, ethyl methyl ester 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, ethyl methyl ester, (.+/-.)- BAY e 5009 Bayotensin Baypress Bylotensin Deiten Ethyl methyl 1,4-dihydro-2,6-dimethyl-4-(m-nitrophenyl)-3,5-pyridinedicarboxylate Nidrel
Inchi:	InChI=1S/C18H20N2O6/c1-5-26-18(22)15-11(3)19-10(2)14(17(21)25-4)16(15)12-7-6-8-1
InchiKey:	PVHUJELLJLJGLN-UHFFFAOYSA-N
Formula:	C18H20N2O6
SMILES:	CCOC(=O)C1=C(C)NC(C)=C(C(=O)OC)C1c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	360.36
CAS:	39562-70-4

Physical Properties

Property code	Value	Unit	Source
gf	-95.27	kJ/mol	Joback Method
hf	-528.34	kJ/mol	Joback Method
hfus	55.28	kJ/mol	Joback Method
hvap	103.92	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	2.566		Crippen Method
mcvol	263.540	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2659.11		NIST Webbook
rinpol	2659.11		NIST Webbook
tb	1033.66	K	Joback Method
tc	1284.55	K	Joback Method
tf	783.50	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.50	J/mol×K	1033.66	Joback Method
cpg	846.15	J/mol×K	1075.48	Joback Method
cpg	852.97	J/mol×K	1117.29	Joback Method
cpg	857.94	J/mol×K	1159.11	Joback Method
cpg	861.05	J/mol×K	1200.92	Joback Method
cpg	862.30	J/mol×K	1242.74	Joback Method
cpg	861.67	J/mol×K	1284.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39562704&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

vc: Critical Volume