Nisoldipine

Other names:	3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-, methyl 2-methylpropyl ester BAY-k 5552 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-, methyl 2-methylpropyl ester, (.+/-.)- (.+/-.)-Isobutyl methyl 1,4-dihydro-2,6-dimethyl-4-(o-nitrophenyl)-3,5-pyridinedicarboxylate 1,4-Dihydro-2,6-dimethyl-4-(2-nitrophenyl)-3,5-pyridinedicarboxylic acid methyl 2-methylpropyl ester Baymycard Nisocor Sular Syscor Zadipina (.+/-.)-Nisoldipine
Inchi:	InChI=1S/C20H24N2O6/c1-11(2)10-28-20(24)17-13(4)21-12(3)16(19(23)27-5)18(17)14-8
InchiKey:	VKQFCGNPDRICFG-UHFFFAOYSA-N
Formula:	C20H24N2O6
SMILES:	COC(=O)C1=C(C)NC(C)=C(C(=O)OCC(C)C)C1c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	388.41
CAS:	63675-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-80.87	kJ/mol	Joback Method
hf	-574.90	kJ/mol	Joback Method
hfus	56.93	kJ/mol	Joback Method
hvap	107.99	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	3.202		Crippen Method
mcvol	291.720	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2679.00		NIST Webbook
tb	1078.98	K	Joback Method
tc	1331.30	K	Joback Method
tf	791.04	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.57	J/mol×K	1078.98	Joback Method
cpg	961.69	J/mol×K	1121.03	Joback Method
cpg	967.83	J/mol×K	1163.09	Joback Method
cpg	971.99	J/mol×K	1205.14	Joback Method
cpg	974.15	J/mol×K	1247.19	Joback Method
cpg	974.34	J/mol×K	1289.25	Joback Method
cpg	972.55	J/mol×K	1331.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C63675729&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