GALLOPAMIL, M(N-BIS-DESALKYL-), AC

Inchi: InChI=1S/C19H28N2O4/c1-13(2)19(12-20,8-7-9-21-14(3)22)15-10-16(23-4)18(25-6)17(1
InchiKey: FDGIVHXEKCWGFY-UHFFFAOYSA-N
Formula: C19H28N2O4
SMILES: COc1cc(C(C#N)(CCCN=C(C)O)C(C)C)cc(OC)c1OC
Mol. weight [g/mol]: 348.44

Physical Properties

Property code	Value	Unit	Source
hf	-558.98	kJ/mol	Joback Method
hvap	98.25	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.886		Crippen Method
mcvol	285.350	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	1010.15	K	Joback Method
tc	1238.38	K	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=R255122&Units=SI

Legend

hf: Enthalpy of formation 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