Gallopamil

Other names:	5-[(3,4-Dimethoxyphenethyl)methylamino]-2-isopropyl-2-(3,4,5-trimethoxyphenyl)valeroni Methoxyverapamil D-600
Inchi:	InChI=1S/C28H40N2O5/c1-20(2)28(19-29,22-17-25(33-6)27(35-8)26(18-22)34-7)13-9-14
InchiKey:	XQLWNAFCTODIRK-UHFFFAOYSA-N
Formula:	C28H40N2O5
SMILES:	COc1ccc(CCN(C)CCCC(C#N)(c2cc(OC)c(OC)c(OC)c2)C(C)C)cc1OC
Mol. weight [g/mol]:	484.63
CAS:	16662-47-8

Physical Properties

Property code	Value	Unit	Source
gf	80.91	kJ/mol	Joback Method
hf	-648.26	kJ/mol	Joback Method
hfus	53.94	kJ/mol	Joback Method
hvap	108.67	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.102		Crippen Method
mcvol	398.570	ml/mol	McGowan Method
pc	863.02	kPa	Joback Method
rinpol	3190.00		NIST Webbook
tb	1141.25	K	Joback Method
tc	1399.88	K	Joback Method
tf	716.79	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1371.59	J/mol×K	1141.25	Joback Method
cpg	1381.79	J/mol×K	1184.36	Joback Method
cpg	1389.57	J/mol×K	1227.46	Joback Method
cpg	1394.95	J/mol×K	1270.57	Joback Method
cpg	1397.97	J/mol×K	1313.67	Joback Method

cpg	1398.67	J/mol×K	1356.78	Joback Method
cpg	1397.08	J/mol×K	1399.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16662478&Units=SI
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

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

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