

VERAPAMIL, M(NOR-), AC

Inchi:	InChI=1S/C28H38N2O5/c1-20(2)28(19-29,23-10-12-25(33-5)27(18-23)35-7)14-8-15-30(2
InchiKey:	GICAVWWNADVQFI-UHFFFAOYSA-N
Formula:	C28H38N2O5
SMILES:	COc1ccc(CCN(CCCC(C#N)(c2ccc(OC)c(OC)c2)C(C)C)C(C)=O)cc1OC
Mol. weight [g/mol]:	482.61

Physical Properties

Property code	Value	Unit	Source
gf	66.62	kJ/mol	Joback Method
hf	-617.15	kJ/mol	Joback Method
hfus	54.74	kJ/mol	Joback Method
hvap	112.34	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.010		Crippen Method
mcvol	394.270	ml/mol	McGowan Method
pc	913.29	kPa	Joback Method
rinsol	3200.00		NIST Webbook
tb	1167.72	K	Joback Method
tc	1432.49	K	Joback Method
tf	731.97	K	Joback Method
vc	1.492	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1351.50	J/molxK	1167.72	Joback Method
cpg	1361.08	J/molxK	1211.85	Joback Method
cpg	1368.51	J/molxK	1255.98	Joback Method
cpg	1373.87	J/molxK	1300.11	Joback Method
cpg	1377.24	J/molxK	1344.24	Joback Method
cpg	1378.70	J/molxK	1388.36	Joback Method
cpg	1378.31	J/molxK	1432.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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