Norverapamil

Other names: Benzeneacetonitrile, «alpha»-[3-[[2-(3,4-dimethoxyphenyl)ethyl]amino]propyl]-3,4-dimethoxy-«alpha»-(1-methy
67812-42-4 (chloride)
5-[(3,4-dimethoxyphenethyl)amino]-2-(3,4-dimethoxyphenyl)-2-isopropylvaleronitrile
Inchi: InChI=1S/C26H36N2O4/c1-19(2)26(18-27,21-9-11-23(30-4)25(17-21)32-6)13-7-14-28-15
InchiKey: UPKQNCPKPOLASS-UHFFFAOYSA-N
Formula: C26H36N2O4
SMILES: COc1ccc(CCNCCCC(C#N)(c2ccc(OC)c(OC)c2)C(C)C)cc1OC
Mol. weight [g/mol]: 440.57
CAS: 67018-85-3

Physical Properties

Property code	Value	Unit	Source
gf	157.31	kJ/mol	Joback Method
hf	-477.35	kJ/mol	Joback Method
hfus	50.04	kJ/mol	Joback Method
hvap	105.54	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.751		Crippen Method
mcvol	364.520	ml/mol	McGowan Method
pc	998.28	kPa	Joback Method
tb	1105.82	K	Joback Method
tc	1353.84	K	Joback Method
tf	679.69	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.44	J/mol×K	1105.82	Joback Method
cpg	1249.54	J/mol×K	1147.16	Joback Method
cpg	1258.70	J/mol×K	1188.49	Joback Method
cpg	1265.96	J/mol×K	1229.83	Joback Method
cpg	1271.37	J/mol×K	1271.16	Joback Method
cpg	1274.97	J/mol×K	1312.50	Joback Method

cpg	1276.80	J/mol×K	1353.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67018853&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume