GALLOPAMIL, M(NOR-), AC

Inchi: InChI=1S/C29H40N2O6/c1-20(2)29(19-30,23-17-26(35-6)28(37-8)27(18-23)36-7)13-9-14
InchiKey: BWALSGMXGXBBJT-UHFFFAOYSA-N
Formula: C29H40N2O6
SMILES: COc1ccc(CCN(CCCC(C#N)(c2cc(OC)c(OC)c(OC)c2)C(C)C)C(C)=O)cc1OC
Mol. weight [g/mol]: 512.64

Physical Properties

Property code	Value	Unit	Source
gf	-39.59	kJ/mol	Joback Method
hf	-781.48	kJ/mol	Joback Method
hfus	58.13	kJ/mol	Joback Method
hvap	117.64	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.018		Crippen Method
mcvol	414.230	ml/mol	McGowan Method
pc	846.53	kPa	Joback Method
rinpol	3520.00		NIST Webbook
tb	1218.00	K	Joback Method
tc	1502.22	K	Joback Method
tf	777.99	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1428.33	J/mol×K	1218.00	Joback Method
cpg	1434.29	J/mol×K	1265.37	Joback Method
cpg	1437.28	J/mol×K	1312.74	Joback Method
cpg	1437.36	J/mol×K	1360.11	Joback Method
cpg	1434.57	J/mol×K	1407.48	Joback Method
cpg	1428.97	J/mol×K	1454.85	Joback Method
cpg	1420.61	J/mol×K	1502.22	Joback Method

Sources

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=R255142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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