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

Inchi: InChI=1S/C18H26N2O3/c1-13(2)18(12-19,9-6-10-20-14(3)21)15-7-8-16(22-4)17(11-15)2
InchiKey: WGTGRACGOFYLKN-UHFFFAOYSA-N
Formula: C18H26N2O3
SMILES: COc1ccc(C(C#N)(CCCNC(C)=O)C(C)C)cc1OC
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	77.88	kJ/mol	Joback Method
hf	-373.96	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	86.06	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.037		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2545.00		NIST Webbook
tb	895.17	K	Joback Method
tc	1113.66	K	Joback Method
tf	543.54	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.52	J/mol×K	895.17	Joback Method
cpg	842.16	J/mol×K	931.58	Joback Method
cpg	854.66	J/mol×K	968.00	Joback Method
cpg	866.08	J/mol×K	1004.41	Joback Method
cpg	876.45	J/mol×K	1040.83	Joback Method
cpg	885.81	J/mol×K	1077.24	Joback Method
cpg	894.19	J/mol×K	1113.66	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=R389889&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