VERAPAMIL, M (N-DESALKYL-), AC

Inchi: InChI=1S/C19H28N2O3/c1-14(2)19(13-20,10-7-11-21(4)15(3)22)16-8-9-17(23-5)18(12-1
InchiKey: DGULUWIIPPFDIS-UHFFFAOYSA-N
Formula: C19H28N2O3
SMILES: COc1ccc(C(C#N)(CCCN(C)C(C)=O)C(C)C)cc1OC
Mol. weight [g/mol]: 332.44

Physical Properties

Property code	Value	Unit	Source
gf	107.69	kJ/mol	Joback Method
hf	-380.54	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	83.89	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.380		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2460.00		NIST Webbook
tb	880.32	K	Joback Method
tc	1094.72	K	Joback Method
tf	534.62	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.60	J/mol×K	880.32	Joback Method
cpg	887.30	J/mol×K	916.05	Joback Method
cpg	900.88	J/mol×K	951.79	Joback Method
cpg	913.37	J/mol×K	987.52	Joback Method
cpg	924.82	J/mol×K	1023.25	Joback Method
cpg	935.29	J/mol×K	1058.99	Joback Method
cpg	944.81	J/mol×K	1094.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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