GALLOPAMIL, M(N-DESALKYL-), AC

Inchi: InChI=1S/C20H30N2O4/c1-14(2)20(13-21,9-8-10-22(4)15(3)23)16-11-17(24-5)19(26-7)1
InchiKey: DVQRRYVJSUQAEL-UHFFFAOYSA-N
Formula: C20H30N2O4
SMILES: COc1cc(C(C#N)(CCCN(C)C(C)=O)C(C)C)cc(OC)c1OC
Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	1.48	kJ/mol	Joback Method
hf	-544.87	kJ/mol	Joback Method
hfus	39.18	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.388		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	930.60	K	Joback Method
tc	1147.32	K	Joback Method
tf	580.64	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.53	J/mol×K	930.60	Joback Method
cpg	972.65	J/mol×K	966.72	Joback Method
cpg	985.50	J/mol×K	1002.84	Joback Method
cpg	997.10	J/mol×K	1038.96	Joback Method
cpg	1007.48	J/mol×K	1075.08	Joback Method
cpg	1016.67	J/mol×K	1111.20	Joback Method
cpg	1024.70	J/mol×K	1147.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255137&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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