Nadolol, N-methyl-, trimethyl ether

Inchi: InChI=1S/C21H35NO4/c1-21(2,3)22(4)13-16(23-5)14-26-18-10-8-9-15-11-19(24-6)20(25
InchiKey: DENMCGUBHQWEEP-UHFFFAOYSA-N
Formula: C21H35NO4
SMILES: COC(COc1cccc2c1CC(OC)C(OC)C2)CN(C)C(C)(C)C
Mol. weight [g/mol]: 365.51

Physical Properties

Property code	Value	Unit	Source
gf	-48.79	kJ/mol	Joback Method
hf	-692.26	kJ/mol	Joback Method
hfus	37.35	kJ/mol	Joback Method
hvap	75.72	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.939		Crippen Method
mcvol	305.590	ml/mol	McGowan Method
pc	1227.70	kPa	Joback Method
rinpol	2523.80		NIST Webbook
rinpol	2523.80		NIST Webbook
tb	821.31	K	Joback Method
tc	1025.74	K	Joback Method
tf	496.88	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.94	J/mol×K	821.31	Joback Method
cpg	1010.89	J/mol×K	855.38	Joback Method
cpg	1029.43	J/mol×K	889.45	Joback Method
cpg	1046.61	J/mol×K	923.52	Joback Method
cpg	1062.44	J/mol×K	957.59	Joback Method
cpg	1076.98	J/mol×K	991.67	Joback Method
cpg	1090.25	J/mol×K	1025.74	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=U333847&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