Alprenolol, N-methyl-, methyl ether

Inchi: InChI=1S/C17H27NO2/c1-6-9-15-10-7-8-11-17(15)20-13-16(19-5)12-18(4)14(2)3/h6-8,10
InchiKey: CPMWAIVHOZZHFS-UHFFFAOYSA-N
Formula: C17H27NO2
SMILES: C=CCc1ccccc1OCC(CN(C)C(C)C)OC
Mol. weight [g/mol]: 277.40

Physical Properties

Property code	Value	Unit	Source
gf	178.78	kJ/mol	Joback Method
hf	-251.19	kJ/mol	Joback Method
hfus	30.51	kJ/mol	Joback Method
hvap	61.79	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.149		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1863.90		NIST Webbook
rinpol	1863.90		NIST Webbook
tb	673.10	K	Joback Method
tc	866.72	K	Joback Method
tf	365.46	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.85	J/mol×K	673.10	Joback Method
cpg	695.61	J/mol×K	705.37	Joback Method
cpg	713.34	J/mol×K	737.64	Joback Method
cpg	730.05	J/mol×K	769.91	Joback Method
cpg	745.78	J/mol×K	802.18	Joback Method
cpg	760.56	J/mol×K	834.45	Joback Method
cpg	774.41	J/mol×K	866.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333826&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