Spiroxamine, isomer 2

Inchi: InChI=1S/C18H35NO2/c1-6-12-19(7-2)13-16-14-20-18(21-16)10-8-15(9-11-18)17(3,4)5/h
InchiKey: PUYXTUJWRLOUCW-UHFFFAOYSA-N
Formula: C18H35NO2
SMILES: CCCN(CC)CC1COC2(CCC(C(C)(C)C)CC2)O1
Mol. weight [g/mol]: 297.48

Physical Properties

Property code	Value	Unit	Source
gf	101.96	kJ/mol	Joback Method
hf	-504.21	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.066		Crippen Method
mcvol	264.480	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	1949.00		NIST Webbook
rinpol	1948.00		NIST Webbook
tb	700.48	K	Joback Method
tc	908.83	K	Joback Method
tf	422.11	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.03	J/mol×K	700.48	Joback Method
cpg	854.02	J/mol×K	735.20	Joback Method
cpg	876.74	J/mol×K	769.93	Joback Method
cpg	898.36	J/mol×K	804.65	Joback Method
cpg	919.03	J/mol×K	839.38	Joback Method
cpg	938.93	J/mol×K	874.10	Joback Method
cpg	958.21	J/mol×K	908.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R566279&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