Paroxetine

Other names:	Piperidine, 3-[(1,3-benzodioxol-5-yloxy)methyl]-4-(4-fluorophenyl)-, (3S-trans)- (-)-(3S,4R)-4-(p-Fluorophenyl)-3-[((3,4-methylenedioxy)phenoxy]methyl]piperidine Aropax BRL-29060 FG-7051 Paxil 3-[(1,3-Benzodioxol-5-yloxy)methyl]-4-(4-fluorophenyl)piperidine, (-)-(3S,4R)- Casbol Frosinor Motivan Paxetil PaxPar Piperidine, 3-((1,3-benzodioxol-5-yloxy)methyl)-4-(4-fluorophenyl)-, (3S,4R)-
Inchi:	InChI=1S/C19H20FNO3/c20-15-3-1-13(2-4-15)17-7-8-21-10-14(17)11-22-16-5-6-18-19(9
InchiKey:	AHOUBRCZNHFOSL-UHFFFAOYSA-N
Formula:	C19H20FNO3
SMILES:	Fc1ccc(C2CCNCC2COc2ccc3c(c2)OCO3)cc1
Mol. weight [g/mol]:	329.37
CAS:	61869-08-7

Physical Properties

Property code	Value	Unit	Source
gf	5.89	kJ/mol	Joback Method
hf	-424.24	kJ/mol	Joback Method
hfus	51.67	kJ/mol	Joback Method
hvap	82.14	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.326		Crippen Method
mcvol	238.690	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	2673.50		NIST Webbook
rinpol	2673.50		NIST Webbook
tb	852.85	K	Joback Method
tc	1103.60	K	Joback Method
tf	600.60	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.16	J/mol×K	852.85	Joback Method
cpg	778.10	J/mol×K	894.64	Joback Method
cpg	793.47	J/mol×K	936.43	Joback Method
cpg	807.36	J/mol×K	978.22	Joback Method
cpg	819.84	J/mol×K	1020.02	Joback Method
cpg	831.01	J/mol×K	1061.81	Joback Method
cpg	840.96	J/mol×K	1103.60	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61869087&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

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