Citalopram

Other names:	Celexa
	5-Isobenzofurancarbonitrile, 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-
	1-[3-(Dimethylamino)propyl]-1-(p-fluorophenyl)-5-phthalancarbonitrile
	Bonitrile
	LU-10-171
	Nitalapram
Inchi:	InChI=1S/C20H21FN2O/c1-23(2)11-3-10-20(17-5-7-18(21)8-6-17)19-9-4-15(13-22)12-16
InchiKey:	WSEQXVZVJXJVFP-UHFFFAOYSA-N
Formula:	C20H21FN2O
SMILES:	CN(C)CCCC1(c2ccc(F)cc2)OCc2cc(C#N)ccc21
Mol. weight [g/mol]:	324.39
CAS:	59729-33-8

Physical Properties

Property code	Value	Unit	Source
gf	331.74	kJ/mol	Joback Method
hf	-25.14	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	81.63	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.813		Crippen Method
mcvol	253.280	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
tb	873.02	K	Joback Method
tc	1106.65	K	Joback Method
tf	572.02	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.18	J/mol×K	873.02	Joback Method
cpg	795.08	J/mol×K	911.96	Joback Method
cpg	811.84	J/mol×K	950.90	Joback Method

cpg	828.70	J/mol×K	989.84	Joback Method
cpg	845.87	J/mol×K	1028.77	Joback Method
cpg	863.58	J/mol×K	1067.71	Joback Method
cpg	882.05	J/mol×K	1106.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59729338&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume