Fluoxetine, N-acetyl

Other names:	Fluoxetin, acetyl
	Fluoxetine, acetyl
Inchi:	InChI=1S/C19H20F3NO2/c1-14(24)23(2)13-12-18(15-6-4-3-5-7-15)25-17-10-8-16(9-11-1
InchiKey:	VFRCUAKESBDNII-UHFFFAOYSA-N
Formula:	C19H20F3NO2
SMILES:	CC(=O)N(C)CCC(Oc1ccc(C(F)(F)F)cc1)c1ccccc1
Mol. weight [g/mol]:	351.36
CAS:	202122-33-6

Physical Properties

Property code	Value	Unit	Source
gf	-382.88	kJ/mol	Joback Method
hf	-753.53	kJ/mol	Joback Method
hfus	36.77	kJ/mol	Joback Method
hvap	70.17	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.694		Crippen Method
mcvol	253.780	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	775.33	K	Joback Method
tc	984.76	K	Joback Method
tf	463.07	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.65	J/mol×K	775.33	Joback Method
cpg	763.01	J/mol×K	810.24	Joback Method
cpg	777.22	J/mol×K	845.14	Joback Method
cpg	790.34	J/mol×K	880.05	Joback Method
cpg	802.45	J/mol×K	914.95	Joback Method

cpg	813.64	J/mol×K	949.86	Joback Method
cpg	823.97	J/mol×K	984.76	Joback Method

Sources

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=C202122336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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