Fluoxetin, nor, acetyl

Inchi: InChI=1S/C18H18F3NO2/c1-13(23)22-12-11-17(14-5-3-2-4-6-14)24-16-9-7-15(8-10-16)1
InchiKey: DNBFECWJDQRKGG-UHFFFAOYSA-N
Formula: C18H18F3NO2
SMILES: CC(=O)NCCC(Oc1ccc(C(F)(F)F)cc1)c1ccccc1
Mol. weight [g/mol]: 337.34

Physical Properties

Property code	Value	Unit	Source
gf	-412.69	kJ/mol	Joback Method
hf	-746.95	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.352		Crippen Method
mcvol	239.690	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
tb	790.18	K	Joback Method
tc	1004.29	K	Joback Method
tf	471.99	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.73	J/mol×K	790.18	Joback Method
cpg	720.93	J/mol×K	825.86	Joback Method
cpg	734.02	J/mol×K	861.55	Joback Method
cpg	746.05	J/mol×K	897.23	Joback Method
cpg	757.11	J/mol×K	932.92	Joback Method
cpg	767.26	J/mol×K	968.60	Joback Method
cpg	776.58	J/mol×K	1004.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R195961&Units=SI

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