Sertraline (ketone), enol, acetyl

Inchi: InChI=1S/C18H14Cl2O2/c1-11(21)22-18-9-7-13(14-4-2-3-5-15(14)18)12-6-8-16(19)17(20
InchiKey: WECDGJVDWWOLEI-CYBMUJFWSA-N
Formula: C18H14Cl2O2
SMILES: CC(=O)OC1=CCC(c2ccc(Cl)c(Cl)c2)c2ccccc21
Mol. weight [g/mol]: 333.21

Physical Properties

Property code	Value	Unit	Source
gf	107.81	kJ/mol	Joback Method
hf	-139.53	kJ/mol	Joback Method
hfus	37.34	kJ/mol	Joback Method
hvap	81.17	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.433		Crippen Method
mcvol	233.720	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	2530.00		NIST Webbook
tb	845.84	K	Joback Method
tc	1100.14	K	Joback Method
tf	542.72	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.58	J/mol×K	845.84	Joback Method
cpg	643.79	J/mol×K	888.22	Joback Method
cpg	655.78	J/mol×K	930.61	Joback Method
cpg	666.65	J/mol×K	972.99	Joback Method
cpg	676.48	J/mol×K	1015.38	Joback Method
cpg	685.35	J/mol×K	1057.76	Joback Method
cpg	693.34	J/mol×K	1100.14	Joback Method
dvisc	0.0007843	Pa×s	542.72	Joback Method
dvisc	0.0005571	Pa×s	593.24	Joback Method

dvisc	0.0004175	Pa×s	643.76	Joback Method
dvisc	0.0003263	Pa×s	694.28	Joback Method
dvisc	0.0002637	Pa×s	744.80	Joback Method
dvisc	0.0002190	Pa×s	795.32	Joback Method
dvisc	0.0001859	Pa×s	845.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R196088&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
dvisc:	Dynamic viscosity
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