Sertraline, (hydroxyketone), acetyl

Inchi: InChI=1S/C18H14Cl2O3/c1-10(21)23-17-9-14(11-6-7-15(19)16(20)8-11)12-4-2-3-5-13(12
InchiKey: UXOKKONDIDHNRH-XPCCGILXSA-N
Formula: C18H14Cl2O3
SMILES: CC(=O)OC1CC(c2ccc(Cl)c(Cl)c2)c2ccccc2C1=O
Mol. weight [g/mol]: 349.21

Physical Properties

Property code	Value	Unit	Source
gf	-42.82	kJ/mol	Joback Method
hf	-343.88	kJ/mol	Joback Method
hfus	37.09	kJ/mol	Joback Method
hvap	84.15	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.643		Crippen Method
mcvol	239.590	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	2660.00		NIST Webbook
tb	904.85	K	Joback Method
tc	1165.37	K	Joback Method
tf	593.42	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.73	J/mol×K	904.85	Joback Method
cpg	700.29	J/mol×K	948.27	Joback Method
cpg	711.24	J/mol×K	991.69	Joback Method
cpg	720.62	J/mol×K	1035.11	Joback Method
cpg	728.45	J/mol×K	1078.53	Joback Method
cpg	734.76	J/mol×K	1121.95	Joback Method
cpg	739.58	J/mol×K	1165.37	Joback Method

Sources

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=R196053&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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