Sertraline, acetyl

Inchi: InChI=1S/C19H19Cl2NO/c1-12(23)22(2)19-10-8-14(15-5-3-4-6-16(15)19)13-7-9-17(20)1
InchiKey: VVNSLNBJUXUABM-LIRRHRJNSA-N
Formula: C19H19Cl2NO
SMILES: CC(=O)N(C)C1CCC(c2ccc(Cl)c(Cl)c2)c2ccccc21
Mol. weight [g/mol]: 348.27

Physical Properties

Property code	Value	Unit	Source
gf	303.97	kJ/mol	Joback Method
hf	-27.07	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	81.76	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.438		Crippen Method
mcvol	256.220	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	849.93	K	Joback Method
tc	1097.05	K	Joback Method
tf	546.71	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.99	J/mol×K	849.93	Joback Method
cpg	750.37	J/mol×K	891.12	Joback Method
cpg	764.47	J/mol×K	932.30	Joback Method
cpg	777.39	J/mol×K	973.49	Joback Method
cpg	789.27	J/mol×K	1014.68	Joback Method
cpg	800.21	J/mol×K	1055.86	Joback Method
cpg	810.33	J/mol×K	1097.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R196048&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
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