Sertraline, nor, acetyl

Inchi: InChI=1S/C18H17Cl2NO/c1-11(22)21-18-9-7-13(14-4-2-3-5-15(14)18)12-6-8-16(19)17(2
InchiKey: YIQKGDBXOASLSF-UGSOOPFHSA-N
Formula: C18H17Cl2NO
SMILES: CC(=O)NC1CCC(c2ccc(Cl)c(Cl)c2)c2ccccc21
Mol. weight [g/mol]: 334.24

Physical Properties

Property code	Value	Unit	Source
gf	274.16	kJ/mol	Joback Method
hf	-20.49	kJ/mol	Joback Method
hfus	41.49	kJ/mol	Joback Method
hvap	83.93	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.096		Crippen Method
mcvol	242.130	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	2700.00		NIST Webbook
tb	864.78	K	Joback Method
tc	1117.11	K	Joback Method
tf	555.63	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.11	J/mol×K	864.78	Joback Method
cpg	705.29	J/mol×K	906.83	Joback Method
cpg	718.23	J/mol×K	948.89	Joback Method
cpg	730.02	J/mol×K	990.94	Joback Method
cpg	740.78	J/mol×K	1033.00	Joback Method
cpg	750.61	J/mol×K	1075.05	Joback Method
cpg	759.62	J/mol×K	1117.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R196093&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