Sertraline (hydroxyketone), (-H2O), enol, acetyl

Inchi: InChI=1S/C18H12Cl2O2/c1-11(21)22-18-9-7-13(14-4-2-3-5-15(14)18)12-6-8-16(19)17(20

InchiKey: HZUSMBBZSXDOPG-UHFFFAOYSA-N

Formula: C18H12Cl2O2

SMILES: CC(=O)Oc1ccc(-c2ccc(Cl)c(Cl)c2)c2ccccc12

Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	135.85	kJ/mol	Joback Method
hf	-72.88	kJ/mol	Joback Method
hfus	37.10	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	5.739		Crippen Method
mcvol	229.420	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	2600.00		NIST Webbook
tb	854.65	K	Joback Method
tc	1111.41	K	Joback Method
tf	560.24	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.98	J/mol×K	854.65	Joback Method
cpg	645.48	J/mol×K	1068.62	Joback Method
cpg	637.32	J/mol×K	1025.82	Joback Method
cpg	628.39	J/mol×K	983.03	Joback Method
cpg	618.58	J/mol×K	940.24	Joback Method
cpg	607.81	J/mol×K	897.44	Joback Method
cpg	652.94	J/mol×K	1111.41	Joback Method
dvisc	0.0001588	Pa×s	854.65	Joback Method
dvisc	0.0001868	Pa×s	805.58	Joback Method

dvisc	0.0002245	Pa×s	756.51	Joback Method
dvisc	0.0002767	Pa×s	707.44	Joback Method
dvisc	0.0003518	Pa×s	658.38	Joback Method
dvisc	0.0004650	Pa×s	609.31	Joback Method
dvisc	0.0006453	Pa×s	560.24	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=R196068&Units=SI

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