Sertraline, ketone

Inchi: InChI=1S/C16H12Cl2O/c17-14-7-5-10(9-15(14)18)11-6-8-16(19)13-4-2-1-3-12(11)13/h1-
InchiKey: JGMBHJNMQVKDMW-LLVKDONJSA-N
Formula: C16H12Cl2O
SMILES: O=C1CCC(c2ccc(Cl)c(Cl)c2)c2ccccc21
Mol. weight [g/mol]: 291.17

Physical Properties

Property code	Value	Unit	Source
gf	181.97	kJ/mol	Joback Method
hf	-37.46	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	70.85	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.102		Crippen Method
mcvol	203.970	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	2480.00		NIST Webbook
tb	787.47	K	Joback Method
tc	1060.11	K	Joback Method
tf	502.96	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.55	J/mol×K	787.47	Joback Method
cpg	552.57	J/mol×K	832.91	Joback Method
cpg	566.13	J/mol×K	878.35	Joback Method
cpg	578.30	J/mol×K	923.79	Joback Method
cpg	589.16	J/mol×K	969.23	Joback Method
cpg	598.77	J/mol×K	1014.67	Joback Method
cpg	607.22	J/mol×K	1060.11	Joback Method

Sources

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=R196073&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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