Zotepine HYAC

Inchi: InChI=1S/C16H11ClO2S/c1-10(18)19-14-8-11-4-2-3-5-15(11)20-16-7-6-12(17)9-13(14)1
InchiKey: NHVDHFRAGVHRTM-UHFFFAOYSA-N
Formula: C16H11ClO2S
SMILES: CC(=O)OC1=Cc2ccccc2Sc2ccc(Cl)cc21
Mol. weight [g/mol]: 302.77

Physical Properties

Property code	Value	Unit	Source
gf	162.57	kJ/mol	Joback Method
hf	-10.75	kJ/mol	Joback Method
hfus	32.65	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.866		Crippen Method
mcvol	209.650	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	2440.00		NIST Webbook
tb	810.88	K	Joback Method
tc	1074.86	K	Joback Method
tf	581.47	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.93	J/mol×K	810.88	Joback Method
cpg	546.04	J/mol×K	854.88	Joback Method
cpg	557.14	J/mol×K	898.87	Joback Method
cpg	567.35	J/mol×K	942.87	Joback Method
cpg	576.79	J/mol×K	986.87	Joback Method
cpg	585.55	J/mol×K	1030.86	Joback Method
cpg	593.76	J/mol×K	1074.86	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=R331310&Units=SI

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