

Zotepine

Inchi:	InChI=1S/C18H18ClNOS/c1-20(2)9-10-21-16-11-13-5-3-4-6-17(13)22-18-8-7-14(19)12-1
InchiKey:	HDOZVRUNCMBHFH-UHFFFAOYSA-N
Formula:	C18H18ClNOS
SMILES:	CN(C)CCOC1=CC2CCCCC2Sc2ccc(Cl)cc21
Mol. weight [g/mol]:	331.87
CAS:	26615-21-4

Physical Properties

Property code	Value	Unit	Source
hfus	39.25	kJ/mol	Joback Method
ie	7.56	eV	Cheméo Relay (1.0)
log10ws	-5.43		Cheméo Relay (1.0)
logp	4.881		Crippen Method
mcvol	246.240	ml/mol	McGowan Method
tf	363.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.29680e+01
Coeff. B	1.52135e+00
Coeff. C	-1.05322e-03
Coeff. D	2.86500e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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