

Sarcolysin

Inchi: InChI=1S/C13H18Cl2N2O2/c14-5-7-17(8-6-15)11-3-1-10(2-4-11)9-12(16)13(18)19/h1-4,11-13,17-19/t14,15,16,17,18,19/s14,15,16,17,18,19
InchiKey: SGDBTWWWUNNDEQ-UHFFFAOYSA-N
Formula: C13H18Cl2N2O2
SMILES: NC(Cc1ccc(N(CCCl)CCCl)cc1)C(=O)O
Mol. weight [g/mol]: 305.20
CAS: 531-76-0

Physical Properties

Property code	Value	Unit	Source
hfus	46.31	kJ/mol	Joback Method
ie	7.74	eV	Cheméo Relay (1.0)
log10ws	-3.45		Cheméo Relay (1.0)
logp	1.925		Crippen Method
mcvol	222.150	ml/mol	McGowan Method
tf	455.65	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	-4.03500e+00
Coeff. B	1.35650e+00
Coeff. C	-9.20160e-04
Coeff. D	2.38000e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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