Phentolamine

Inchi: InChI=1S/C17H19N3O/c1-13-5-7-14(8-6-13)20(12-17-18-9-10-19-17)15-3-2-4-16(21)11-
InchiKey: MRBDMNSDAVCSSF-UHFFFAOYSA-N
Formula: C17H19N3O
SMILES: Cc1ccc(N(CC2=NCCN2)c2cccc(O)c2)cc1
Mol. weight [g/mol]: 281.36
CAS: 50-60-2

Physical Properties

Property code	Value	Unit	Source
hfus	44.71	kJ/mol	Joback Method
log10ws	-3.47		Cheméo Relay (1.0)
logp	2.840		Crippen Method
mcvol	223.520	ml/mol	McGowan Method
tf	447.90	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	-1.06189e+02
Coeff. B	1.74280e+00
Coeff. C	-1.23252e-03
Coeff. D	3.40800e-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):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Joback Method:	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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
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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