

Metipranolol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C17H27NO4/c1-10(2)18-8-15(20)9-21-16-7-11(3)17(22-14(6)19)13(5)12(16)4/

BQIPXWYNLPYNHW-UHFFFAOYSA-N

C17H27NO4

CC(=O)Oc1c(C)cc(OCC(O)CNC(C)C)c(C)c1C

309.41

22664-55-7

Physical Properties

Property code	Value	Unit	Source
hfus	39.97	kJ/mol	Joback Method
log10ws	-1.97		Cheméo Relay (1.0)
logp	2.275		Crippen Method
mcvol	255.790	ml/mol	McGowan Method
tf	379.15		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	6.23520e+01
Coeff. B	1.30602e+00
Coeff. C	-5.43840e-04
Coeff. D	2.44000e-08
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/106-252-4/Metipranolol.pdf>

Generated by Cheméo on 2026-10-31 00:44:17.270486341 +0000 UTC m=+31170.197323624.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.