

Tocainide

Inchi:

InChI=1S/C11H16N2O/c1-7-5-4-6-8(2)10(7)13-11(14)9(3)12/h4-6,9H,12H2,1-3H3,(H,13,

InchiKey:

BUJAGSGYPOAWEI-UHFFFAOYSA-N

Formula:

C11H16N2O

SMILES:

Cc1cccc(C)c1NC(=O)C(C)N

Mol. weight [g/mol]:

192.26

CAS:

41708-72-9

Physical Properties

Property code	Value	Unit	Source
hfus	25.88	kJ/mol	Joback Method
ie	7.83	eV	Cheméo Relay (1.0)
log10ws	-1.64		Cheméo Relay (1.0)
logp	1.589		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
tf	529.15	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	-1.46000e+00
Coeff. B	9.66960e-01
Coeff. C	-5.48220e-04
Coeff. D	1.07360e-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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