

Trimebutine

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C22H29NO5/c1-7-22(23(2)3,17-11-9-8-10-12-17)15-28-21(24)16-13-18(25-4)2

LORDFXWUHHSAQU-UHFFFAOYSA-N

C22H29NO5

CCC(COC(=O)c1cc(OC)c(OC)c(OC)c1)(c1ccccc1)N(C)C

387.48

39133-31-8

Physical Properties

Property code	Value	Unit	Source
hfus	43.19	kJ/mol	Joback Method
logp	3.736		Crippen Method
mcvol	308.350	ml/mol	McGowan Method
tb	680.72	K	Cheméo Relay (1.0)
tf	352.15	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	2.47220e+01
Coeff. B	1.76292e+00
Coeff. C	-8.91080e-04
Coeff. D	1.14700e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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