

Dihydrotachysterol

Inchi:	InChI=1S/C28H46O/c1-19(2)20(3)9-10-22(5)26-15-16-27-23(8-7-17-28(26,27)6)12-13-24
InchiKey:	ILYCWAKSDCYMBB-UHFFFAOYSA-N
Formula:	C28H46O
SMILES:	CC1CCC(O)CC1=CC=C1CCCC2(C)C1CCC2C(C)C=CC(C)C(C)C
Mol. weight [g/mol]:	398.67
CAS:	67-96-9

Physical Properties

Property code	Value	Unit	Source
hfus	40.29	kJ/mol	Joback Method
logp	7.721		Crippen Method
mcvol	365.770	ml/mol	McGowan Method
tf	399.15	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	-2.33870e+02
Coeff. B	3.21462e+00
Coeff. C	-2.36420e-03
Coeff. D	7.39600e-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):
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

Legend

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

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<https://www.chemeo.com/cid/100-056-8/Dihydrotachysterol.pdf>

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