

7,11b-dihydro-6H-indeno[2,1-c]chromene-3,4,6a,9

Inchi:	InChI=1S/C16H14O6/c17-10-2-1-8-13-9-4-12(19)11(18)3-7(9)5-16(13,21)6-22-15(8)14(1
InchiKey:	WZUVPPKBWHMQCE-UHFFFAOYSA-N
Formula:	C16H14O6
SMILES:	Oc1cc2c(cc1O)C1c3ccc(O)c(O)c3OCC1(O)C2
Mol. weight [g/mol]:	302.28
CAS:	517-28-2

Physical Properties

Property code	Value	Unit	Source
hfus	51.77	kJ/mol	Joback Method
logp	1.320		Crippen Method
mcvol	202.280	ml/mol	McGowan Method
tf	413.15	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	-2.09290e+02
Coeff. B	2.49970e+00
Coeff. C	-2.83626e-03
Coeff. D	1.24040e-06
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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