4-[18-(4-hydroxy-2,6,6-trimethylcyclohex-2-en-1-y

Inchi: InChI=1S/C40H56O2/c1-29(17-13-19-31(3)21-23-37-33(5)25-35(41)27-39(37,7)8)15-11-
InchiKey: KBPHJBAIARWVSC-UHFFFAOYSA-N
Formula: C40H56O2
SMILES: CC(C=CC=C(C)C=CC1=C(C)CC(O)CC1(C)C)=CC=CC=C(C)C=CC=C(C)C=CC1C(C)=C
Mol. weight [g/mol]: 568.89
CAS: 127-40-2

Physical Properties

Property code	Value	Unit	Source
hfus	79.67	kJ/mol	Joback Method
ie	6.71	eV	Cheméo Relay (1.0)
logp	10.403		Crippen Method
mcvol	517.180	ml/mol	McGowan Method
tf	466.15	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	-3.04210e+02
Coeff. B	4.50960e+00
Coeff. C	-3.81084e-03
Coeff. D	1.38250e-06
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/ci990307l
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_Datset/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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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