3,3-bis(4-hydroxy-2-methyl-5-propan-2-ylphenyl)-2

Inchi: InChI=1S/C28H30O4/c1-15(2)20-13-23(17(5)11-25(20)29)28(22-10-8-7-9-19(22)27(31)3
InchiKey: LDKDGDIWEUUXSH-UHFFFAOYSA-N
Formula: C28H30O4
SMILES: Cc1cc(O)c(C(C)C)cc1C1(c2cc(C(C)C)c(O)cc2C)OC(=O)c2ccccc21
Mol. weight [g/mol]: 430.54
CAS: 125-20-2

Physical Properties

Property code	Value	Unit	Source
hfus	53.38	kJ/mol	Joback Method
log10ws	-6.38		Cheméo Relay (1.0)
logp	6.424		Crippen Method
mcvol	342.420	ml/mol	McGowan Method
tf	525.15	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	-1.38570e+02
Coeff. B	2.85792e+00
Coeff. C	-2.52792e-03
Coeff. D	9.39200e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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
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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
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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