

6-fluoro-11-hydroxy-17-(2-hydroxyacetyl)-10,13,16

Inchi:	InChI=1S/C22H29FO4/c1-11-6-14-13-8-16(23)15-7-12(25)4-5-21(15,2)20(13)17(26)9-22
InchiKey:	GAKMQHDJQHZUTJ-UHFFFAOYSA-N
Formula:	C22H29FO4
SMILES:	CC1CC2C3CC(F)C4=CC(=O)C=CC4(C)C3C(O)CC2(C)C1C(=O)CO
Mol. weight [g/mol]:	376.47
CAS:	152-97-6

Physical Properties

Property code	Value	Unit	Source
hfus	41.95	kJ/mol	Joback Method
log10ws	-4.22		Cheméo Relay (1.0)
logp	2.637		Crippen Method
mcvol	285.450	ml/mol	McGowan Method
tf	461.15	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	-2.23649e+02
Coeff. B	2.81276e+00
Coeff. C	-2.33202e-03
Coeff. D	8.39960e-07
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
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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