5«alpha»-Androstane-3«beta»,17«beta»-diol, bis(trifluoroacetate)

Inchi: InChI=1S/C23H30F6O4/c1-20-9-7-13(32-18(30)22(24,25)26)11-12(20)3-4-14-15-5-6-17(

InchiKey: NXQFDYRIAIABNB-UHFFFAOYSA-N

Formula: C23H30F6O4

SMILES: CC12CCC(OC(=O)C(F)(F)F)CC1CCC1C2CCC2(C)C(OC(=O)C(F)(F)F)CCC12

Mol. weight [g/mol]: 484.47

Physical Properties

Property code	Value	Unit	Source
hfus	38.28	kJ/mol	Joback Method
logp	5.977		Crippen Method
mcvol	316.990	ml/mol	McGowan Method
rinpol	2375.10		NIST Webbook
rinpol	2375.10		NIST Webbook
tf	388.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.32	J/mol×K	897.49	Joback Method
cpg	1190.15	J/mol×K	933.00	Joback Method
cpg	1214.03	J/mol×K	968.51	Joback Method
cpg	1238.23	J/mol×K	1004.03	Joback Method
cpg	1263.04	J/mol×K	1039.54	Joback Method
cpg	1288.73	J/mol×K	1075.05	Joback Method
cpg	1315.58	J/mol×K	1110.56	Joback Method

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352245&Units=SI

Legend

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