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

Inchi: InChI=1S/C25H30F10O4/c1-20-9-7-13(38-18(36)22(26,27)24(30,31)32)11-12(20)3-4-14-

InchiKey: VGVRMALUWHWDMN-UHFFFAOYSA-N

Formula: C25H30F10O4

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

Mol. weight [g/mol]: 584.49

Physical Properties

Property code	Value	Unit	Source
hfus	40.95	kJ/mol	Joback Method
logp	7.248		Crippen Method
mcvol	352.250	ml/mol	McGowan Method
rinpol	2292.30		NIST Webbook
rinpol	2292.30		NIST Webbook
tf	385.62	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1323.80	J/mol×K	933.87	Joback Method
cpg	1348.14	J/mol×K	969.07	Joback Method
cpg	1372.89	J/mol×K	1004.27	Joback Method
cpg	1398.38	J/mol×K	1039.47	Joback Method
cpg	1424.91	J/mol×K	1074.67	Joback Method
cpg	1452.82	J/mol×K	1109.87	Joback Method
cpg	1482.43	J/mol×K	1145.07	Joback Method

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352241&Units=SI
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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point