Etiocholan-3«alpha»-ol-17-one, pentafluoropropionate

Inchi: InChI=1S/C22H29F5O3/c1-19-9-7-13(30-18(29)21(23,24)22(25,26)27)11-12(19)3-4-14-1

InchiKey: MDOSQUKLWNVMRK-UHFFFAOYSA-N

Formula: C22H29F5O3

SMILES: CC12CCC3C(CCC4CC(OC(=O)C(F)(F)C(F)(F)F)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 436.46

Physical Properties

Property code	Value	Unit	Source
hfus	28.26	kJ/mol	Joback Method
log10ws	-6.36		Cheméo Relay (1.0)
logp	5.708		Crippen Method
mcvol	295.260	ml/mol	McGowan Method
rinpol	2411.20		NIST Webbook
rinpol	2411.20		NIST Webbook
tf	397.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1077.09	J/mol×K	871.54	Joback Method
cpg	1101.49	J/mol×K	908.67	Joback Method
cpg	1125.80	J/mol×K	945.80	Joback Method
cpg	1150.32	J/mol×K	982.93	Joback Method
cpg	1175.37	J/mol×K	1020.07	Joback Method
cpg	1201.25	J/mol×K	1057.20	Joback Method
cpg	1228.26	J/mol×K	1094.33	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=U352246&Units=SI

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point