Androst-5-en-3-ol, trifluoroacetate, (3«beta»)-

Other names: Androst-5-en-3«beta»-ol, TFA
Inchi: InChI=1S/C21H29F3O2/c1-19-9-3-4-16(19)15-6-5-13-12-14(26-18(25)21(22,23)24)7-11-
InchiKey: OGQQARADPATKJB-ZLDOSZBNSA-N
Formula: C21H29F3O2
SMILES: CC12CCCC1C1CC=C3CC(OC(=O)C(F)(F)F)CCC3(C)C1CC2
Mol. weight [g/mol]: 370.45
CAS: 56438-15-4

Physical Properties

Property code	Value	Unit	Source
hfus	27.18	kJ/mol	Joback Method
log10ws	-5.73		Cheméo Relay (1.0)
logp	5.813		Crippen Method
mcvol	271.760	ml/mol	McGowan Method
rinpol	2201.00		NIST Webbook
rinpol	2201.00		NIST Webbook
tf	392.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.10	J/mol×K	794.34	Joback Method
cpg	947.83	J/mol×K	831.51	Joback Method
cpg	971.11	J/mol×K	868.68	Joback Method
cpg	994.26	J/mol×K	905.85	Joback Method
cpg	1017.58	J/mol×K	943.02	Joback Method
cpg	1041.41	J/mol×K	980.19	Joback Method
cpg	1066.06	J/mol×K	1017.36	Joback Method

Sources

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=C56438154&Units=SI
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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point