

Androst-5-en-16-one, 3,17-bis[(trifluoroacetyl)oxy]-, (3«beta»,17«beta»)-

Other names: Androst-5-en-3«beta»,17«beta»-diol-16-one, TFA

Inchi: InChI=1S/C23H26F6O5/c1-20-7-5-12(33-18(31)22(24,25)26)9-11(20)3-4-13-14(20)6-8-2

InchiKey: CTNWZUBGEFFWGH-VPPKIAQMSA-N

Formula: C23H26F6O5

SMILES: CC12CCC(OC(=O)C(F)(F)F)CC1=CCC1C2CCC2(C)C(OC(=O)C(F)(F)F)C(=O)CC12

Mol. weight [g/mol]: 496.44

CAS: 56438-14-3

Physical Properties

Property code	Value	Unit	Source
gf	-1442.11	kJ/mol	Joback Method
hf	-2063.34	kJ/mol	Joback Method
hfus	37.55	kJ/mol	Joback Method
hvap	80.09	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.076		Crippen Method
mcvol	314.260	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
tb	974.12	K	Joback Method
tc	1200.73	K	Joback Method
tf	672.41	K	Joback Method
vc	1.232	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.88	J/molxK	974.12	Joback Method
cpg	1201.34	J/molxK	1011.89	Joback Method
cpg	1226.41	J/molxK	1049.66	Joback Method
cpg	1252.39	J/molxK	1087.43	Joback Method
cpg	1279.57	J/molxK	1125.20	Joback Method
cpg	1308.28	J/molxK	1162.96	Joback Method
cpg	1338.80	J/molxK	1200.73	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56438143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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