

Androst-5-ene-17-carboxylic acid, 3beta-hydroxy-, methyl ester

Inchi:	InChI=1S/C21H32O3/c1-20-10-8-14(22)12-13(20)4-5-15-16-6-7-18(19(23)24-3)21(16,2)
InchiKey:	WGYHVQYXJNPQAA-UHFFFAOYSA-N
Formula:	C21H32O3
SMILES:	COC(=O)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	332.48
CAS:	200263-91-8

Physical Properties

Property code	Value	Unit	Source
gf	-76.08	kJ/mol	Joback Method
hf	-597.63	kJ/mol	Joback Method
hfus	30.51	kJ/mol	Joback Method
hvap	86.41	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.099		Crippen Method
mcvol	272.320	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
tb	887.27	K	Joback Method
tc	1112.74	K	Joback Method
tf	561.93	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.61	J/molxK	887.27	Joback Method
cpg	1007.12	J/molxK	924.85	Joback Method
cpg	1031.85	J/molxK	962.43	Joback Method
cpg	1057.07	J/molxK	1000.01	Joback Method
cpg	1083.09	J/molxK	1037.58	Joback Method
cpg	1110.21	J/molxK	1075.16	Joback Method
cpg	1138.70	J/molxK	1112.74	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C200263918&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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