

5-Androstene-3beta-ol,17-one-16-ylidenacetic acid, 3-acetate

Inchi:	InChI=1S/C23H30O5/c1-13(24)28-16-6-8-22(2)15(12-16)4-5-17-18(22)7-9-23(3)19(17)10
InchiKey:	WFBQLTRVAIINMK-SDNWHVSQSA-N
Formula:	C23H30O5
SMILES:	CC(=O)OC1CCC2(C)C(=CCC3C4CC(=CC(=O)O)C(=O)C4(C)CCC32)C1
Mol. weight [g/mol]:	386.48
CAS:	96708-99-5

Physical Properties

Property code	Value	Unit	Source
gf	-257.58	kJ/mol	Joback Method
hf	-792.82	kJ/mol	Joback Method
hfus	36.05	kJ/mol	Joback Method
hvap	102.95	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.071		Crippen Method
mcvol	299.340	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
tb	1066.03	K	Joback Method
tc	1312.55	K	Joback Method
tf	717.22	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.52	J/mol×K	1066.03	Joback Method
cpg	1183.55	J/mol×K	1107.12	Joback Method
cpg	1215.19	J/mol×K	1148.20	Joback Method
cpg	1248.81	J/mol×K	1189.29	Joback Method
cpg	1284.75	J/mol×K	1230.38	Joback Method
cpg	1323.37	J/mol×K	1271.46	Joback Method
cpg	1365.04	J/mol×K	1312.55	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=C96708995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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