5Alpha-androstone-3beta, 17beta-diol,16-ylacetic acid, 3,17-diacetate

Inchi: InChI=1S/C25H38O6/c1-14(26)30-18-7-9-24(3)17(13-18)5-6-19-20(24)8-10-25(4)21(19)1

InchiKey: ZCECNGOCGUYLHX-UHFFFAOYSA-N

Formula: C25H38O6

SMILES: CC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C3CC(CC(=O)O)C2OC(C)=O)C1

Mol. weight [g/mol]: 434.57

CAS: 125638-43-9

Physical Properties

Property code	Value	Unit	Source
gf	-440.99	kJ/mol	Joback Method
hf	-1124.56	kJ/mol	Joback Method
hfus	46.57	kJ/mol	Joback Method
hvap	109.65	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.593		Crippen Method
mcvol	341.990	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
tb	1095.47	K	Joback Method
tc	1341.39	K	Joback Method
tf	707.34	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1380.02	J/mol×K	1095.47	Joback Method
cpg	1412.56	J/mol×K	1136.46	Joback Method
cpg	1446.49	J/mol×K	1177.44	Joback Method
cpg	1482.16	J/mol×K	1218.43	Joback Method
cpg	1519.93	J/mol×K	1259.41	Joback Method
cpg	1560.17	J/mol×K	1300.40	Joback Method
cpg	1603.21	J/mol×K	1341.39	Joback Method

Sources

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=C125638439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume