

3Beta,17beta-diacetoxy-5alpha-androstan-16-ylid

Inchi:
acid

InChI=1S/C25H36O6/c1-14(26)30-18-7-9-24(3)17(13-18)5-6-19-20(24)8-10-25(4)21(19)

InchiKey:

MFQVPGHQVVZKOB-FOWTUZBSSA-N

Formula:

C25H36O6

SMILES:

CC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(OC(C)=O)C(=CC(=O)O)CC3)C1

Mol. weight [g/mol]:

432.55

CAS:

18039-58-2

Physical Properties

Property code	Value	Unit	Source
gf	-387.82	kJ/mol	Joback Method
hf	-1028.19	kJ/mol	Joback Method
hfus	45.82	kJ/mol	Joback Method
hvap	110.74	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.513		Crippen Method
mcvol	337.690	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
tb	1106.78	K	Joback Method
tc	1355.41	K	Joback Method
tf	721.94	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.77	J/molxK	1106.78	Joback Method
cpg	1381.28	J/molxK	1148.22	Joback Method
cpg	1416.58	J/molxK	1189.66	Joback Method
cpg	1454.04	J/molxK	1231.10	Joback Method
cpg	1494.05	J/molxK	1272.54	Joback Method
cpg	1536.99	J/molxK	1313.97	Joback Method
cpg	1583.24	J/molxK	1355.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C18039582&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
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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