

Pregn-4-ene-3,20-dione,11beta,17alpha,21-trihydr

Inchi:
acetate

InChI=1S/C23H32O6/c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-15(25)6-8-21(14)

InchiKey:

ALEXXDVDDISNDU-UHFFFAOYSA-N

Formula:

C23H32O6

SMILES:

CC(=O)OCC(=O)C1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3C(O)CC21C

Mol. weight [g/mol]:

404.50

CAS:

61376-87-2

Physical Properties

Property code	Value	Unit	Source
gf	-453.06	kJ/mol	Joback Method
hf	-1026.18	kJ/mol	Joback Method
hfus	34.59	kJ/mol	Joback Method
hvap	117.38	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.352		Crippen Method
mcvol	309.510	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
tb	1147.14	K	Joback Method
tc	1404.43	K	Joback Method
tf	787.34	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.14	J/molxK	1147.14	Joback Method
cpg	1354.32	J/molxK	1190.02	Joback Method
cpg	1404.71	J/molxK	1232.90	Joback Method
cpg	1459.86	J/molxK	1275.78	Joback Method
cpg	1520.29	J/molxK	1318.67	Joback Method
cpg	1586.56	J/molxK	1361.55	Joback Method
cpg	1659.18	J/molxK	1404.43	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=C61376872&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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