2Alpha,11beta,17alpha,21-tetrahydroxypregn-4-en

Inchi: InChI=1S/C21H30O6/c1-19-8-15(24)14(23)7-11(19)3-4-12-13-5-6-21(27,17(26)10-22)20...

InchiKey: RORUGVXGZMMYON-UHFFFAOYSA-N

Formula: C21H30O6

SMILES: CC12CC(O)C(=O)C=C1CCC1C2C(O)CC2(C)C1CCC2(O)C(=O)CO

Mol. weight [g/mol]: 378.46

CAS: 520-84-3

Physical Properties

Property code	Value	Unit	Source
gf	-517.33	kJ/mol	Joback Method
hf	-1064.90	kJ/mol	Joback Method
hfus	35.87	kJ/mol	Joback Method
hvap	136.83	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	0.752		Crippen Method
mcvol	285.630	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
tb	1204.78	K	Joback Method
tc	1487.69	K	Joback Method
tf	810.04	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1304.38	J/mol×K	1204.78	Joback Method
cpg	1362.75	J/mol×K	1251.93	Joback Method
cpg	1427.56	J/mol×K	1299.08	Joback Method
cpg	1499.55	J/mol×K	1346.23	Joback Method
cpg	1579.44	J/mol×K	1393.39	Joback Method
cpg	1667.98	J/mol×K	1440.54	Joback Method
cpg	1765.89	J/mol×K	1487.69	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=C520843&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

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