

14Alpha,21-dihydroxypregn-4-ene-3,20-dione

Other names:	14«alpha»-Hydroxydeoxycorticosterone 14Alpha,21-dihydroxypregn-4-ene-3,20-dione
Inchi:	InChI=1S/C21H30O4/c1-19-8-5-14(23)11-13(19)3-4-16-15(19)6-9-20(2)17(18(24)12-22)
InchiKey:	XKCAPZYNIKDWOX-UHFFFAOYSA-N
Formula:	C21H30O4
SMILES:	CC12CCC(=O)C=C1CCC1C2CCC2(C)C(C(=O)CO)CCC12O
Mol. weight [g/mol]:	346.47

Physical Properties

Property code	Value	Unit	Source
hfus	25.55	kJ/mol	Joback Method
log10ws	-3.39		Cheméo Relay (1.0)
logp	2.811		Crippen Method
mcvol	273.890	ml/mol	McGowan Method
tf	480.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1081.15	J/mol×K	1029.76	Joback Method
cpg	1115.41	J/mol×K	1069.49	Joback Method
cpg	1152.45	J/mol×K	1109.22	Joback Method
cpg	1192.71	J/mol×K	1148.94	Joback Method
cpg	1236.66	J/mol×K	1188.67	Joback Method
cpg	1284.74	J/mol×K	1228.40	Joback Method
cpg	1337.41	J/mol×K	1268.13	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C595711&Units=SI>

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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