

16ALPHA,17-EPOXYPROGESTERONE

Other names:	16-«alpha»,17-Epoxy pregn-4-ene-3,20-dione 16«alpha»,17«alpha»-Epoxy pregn-4-ene-3,20-dione 16«alpha»,17«alpha»-epoxyprogesterone Pregn-4-ene-3,20-dione, 16-«alpha»,17-epoxy-
Inchi:	InChI=1S/C21H28O3/c1-12(22)21-18(24-21)11-17-15-5-4-13-10-14(23)6-8-19(13,2)16(1
InchiKey:	LHNVKVKZPHUYQO-UHFFFAOYSA-N
Formula:	C21H28O3
SMILES:	CC(=O)C12OC1CC1C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	328.45

Physical Properties

Property code	Value	Unit	Source
hfus	27.69	kJ/mol	Joback Method
log10ws	-4.55		Cheméo Relay (1.0)
logp	3.855		Crippen Method
mcvol	257.160	ml/mol	McGowan Method
tf	440.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.39	J/mol×K	870.55	Joback Method
cpg	950.56	J/mol×K	913.24	Joback Method
cpg	981.32	J/mol×K	955.93	Joback Method
cpg	1014.29	J/mol×K	998.62	Joback Method
cpg	1050.10	J/mol×K	1041.31	Joback Method
cpg	1089.37	J/mol×K	1084.00	Joback Method
cpg	1132.72	J/mol×K	1126.69	Joback Method
hfust	26.40	kJ/mol	328.50	NIST Webbook

Sources

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=C1097514&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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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