3,17-dimethoxypregna-2,4-dien-20-one

Inchi: InChI=1S/C23H34O3/c1-15(24)23(26-5)13-10-20-18-7-6-16-14-17(25-4)8-11-21(16,2)19
InchiKey: WGMORNSWMKZSGW-UHFFFAOYSA-N
Formula: C23H34O3
SMILES: COC1=CCC2(C)C(=C1)CCC1C2CCC2(C)C1CCC2(OC)C(C)=O
Mol. weight [g/mol]: 358.52

Physical Properties

Property code	Value	Unit	Source
hfus	26.26	kJ/mol	Joback Method
log10ws	-5.15		Cheméo Relay (1.0)
logp	5.064		Crippen Method
mcvol	296.200	ml/mol	McGowan Method
rinpol	2959.60		NIST Webbook
rinpol	2959.60		NIST Webbook
tf	421.79	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.14	J/mol×K	872.32	Joback Method
cpg	1058.14	J/mol×K	911.96	Joback Method
cpg	1088.04	J/mol×K	951.60	Joback Method
cpg	1119.28	J/mol×K	991.24	Joback Method
cpg	1152.31	J/mol×K	1030.88	Joback Method
cpg	1187.58	J/mol×K	1070.52	Joback Method
cpg	1225.52	J/mol×K	1110.16	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333779&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point