Etiocholan-3«alpha»-ol-17-one, acetate

Inchi: InChI=1S/C21H32O3/c1-13(22)24-15-8-10-20(2)14(12-15)4-5-16-17-6-7-19(23)21(17,3)1
InchiKey: FDCINQSOYQUNKB-UHFFFAOYSA-N
Formula: C21H32O3
SMILES: CC(=O)OC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]: 332.48

Physical Properties

Property code	Value	Unit	Source
hfus	25.10	kJ/mol	Joback Method
log10ws	-4.89		Cheméo Relay (1.0)
logp	4.530		Crippen Method
mcvol	272.320	ml/mol	McGowan Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tf	410.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.38	J/mol×K	858.77	Joback Method
cpg	1004.86	J/mol×K	899.67	Joback Method
cpg	1032.08	J/mol×K	940.57	Joback Method
cpg	1059.38	J/mol×K	981.46	Joback Method
cpg	1087.10	J/mol×K	1022.36	Joback Method
cpg	1115.57	J/mol×K	1063.26	Joback Method
cpg	1145.13	J/mol×K	1104.16	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368360&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):	
Cheméo Relay (1.0, beta):	

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