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

Inchi: InChI=1S/C25H40O3/c1-4-5-6-7-23(27)28-18-12-14-24(2)17(16-18)8-9-19-20-10-11-22(2
InchiKey: SMYVCRCXPSLNDH-UHFFFAOYSA-N
Formula: C25H40O3
SMILES: CCCCCC(=O)OC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]: 388.58

Physical Properties

Property code	Value	Unit	Source
hfus	35.46	kJ/mol	Joback Method
log10ws	-6.04		Cheméo Relay (1.0)
logp	6.090		Crippen Method
mcvol	328.680	ml/mol	McGowan Method
rinpol	2544.00		NIST Webbook
rinpol	2544.00		NIST Webbook
tf	389.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1240.37	J/mol×K	950.29	Joback Method
cpg	1270.15	J/mol×K	989.41	Joback Method
cpg	1300.14	J/mol×K	1028.53	Joback Method
cpg	1330.65	J/mol×K	1067.65	Joback Method
cpg	1361.99	J/mol×K	1106.77	Joback Method
cpg	1394.47	J/mol×K	1145.89	Joback Method
cpg	1428.41	J/mol×K	1185.02	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368363&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