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

Inchi: InChI=1S/C27H44O3/c1-4-5-6-7-8-9-25(29)30-20-14-16-26(2)19(18-20)10-11-21-22-12-1
InchiKey: BTEOMWNRKOOBJV-UHFFFAOYSA-N
Formula: C27H44O3
SMILES: CCCCCCCC(=O)OC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]: 416.64

Physical Properties

Property code	Value	Unit	Source
hfus	40.64	kJ/mol	Joback Method
log10ws	-6.70		Cheméo Relay (1.0)
logp	6.870		Crippen Method
mcvol	356.860	ml/mol	McGowan Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tf	387.56	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1378.22	J/mol×K	996.05	Joback Method
cpg	1409.86	J/mol×K	1035.06	Joback Method
cpg	1441.96	J/mol×K	1074.07	Joback Method
cpg	1474.84	J/mol×K	1113.09	Joback Method
cpg	1508.81	J/mol×K	1152.10	Joback Method
cpg	1544.21	J/mol×K	1191.11	Joback Method
cpg	1581.33	J/mol×K	1230.12	Joback Method

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=U368364&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
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