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

Inchi: InChI=1S/C23H36O3/c1-4-5-21(25)26-16-10-12-22(2)15(14-16)6-7-17-18-8-9-20(24)23(1
InchiKey: ZBPQBCXWLUSWGS-UHFFFAOYSA-N
Formula: C23H36O3
SMILES: CCCC(=O)OC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]: 360.53

Physical Properties

Property code	Value	Unit	Source
hfus	30.28	kJ/mol	Joback Method
log10ws	-5.45		Cheméo Relay (1.0)
logp	5.310		Crippen Method
mcvol	300.500	ml/mol	McGowan Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tf	390.59	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1106.74	J/mol×K	904.53	Joback Method
cpg	1135.18	J/mol×K	944.30	Joback Method
cpg	1163.60	J/mol×K	984.07	Joback Method
cpg	1192.31	J/mol×K	1023.83	Joback Method
cpg	1221.63	J/mol×K	1063.60	Joback Method
cpg	1251.89	J/mol×K	1103.37	Joback Method
cpg	1283.39	J/mol×K	1143.14	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368362&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