5-«beta»-cholestan-3«alpha»-ol, propionate

Inchi: InChI=1S/C30H52O2/c1-7-28(31)32-23-15-17-29(5)22(19-23)11-12-24-26-14-13-25(21(4
InchiKey: BZAVPIMVSGSUNL-UHFFFAOYSA-N
Formula: C30H52O2
SMILES: CCC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]: 444.73

Physical Properties

Property code	Value	Unit	Source
gf	103.60	kJ/mol	Joback Method
hf	-708.37	kJ/mol	Joback Method
hfus	42.92	kJ/mol	Joback Method
hvap	87.73	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	8.429		Crippen Method
mcvol	397.560	ml/mol	McGowan Method
pc	848.50	kPa	Joback Method
rinpol	2713.00		NIST Webbook
tb	991.32	K	Joback Method
tc	1219.60	K	Joback Method
tf	555.02	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1537.08	J/mol×K	991.32	Joback Method
cpg	1570.97	J/mol×K	1029.37	Joback Method
cpg	1605.29	J/mol×K	1067.41	Joback Method
cpg	1640.37	J/mol×K	1105.46	Joback Method
cpg	1676.55	J/mol×K	1143.51	Joback Method
cpg	1714.15	J/mol×K	1181.55	Joback Method
cpg	1753.52	J/mol×K	1219.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368376&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume