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

Inchi: InChI=1S/C28H48O2/c1-19(2)7-6-8-20(3)24-11-12-25-23-10-9-21-17-22(30-18-29)13-15
InchiKey: CPSQZDFMYGLDLH-UHFFFAOYSA-N
Formula: C28H48O2
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4CC(OC=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 416.68

Physical Properties

Property code	Value	Unit	Source
gf	116.16	kJ/mol	Joback Method
hf	-640.09	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	83.25	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	7.649		Crippen Method
mcvol	369.380	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	2593.00		NIST Webbook
tb	940.35	K	Joback Method
tc	1164.45	K	Joback Method
tf	524.55	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1393.13	J/mol×K	940.35	Joback Method
cpg	1424.57	J/mol×K	977.70	Joback Method
cpg	1456.12	J/mol×K	1015.05	Joback Method
cpg	1488.08	J/mol×K	1052.40	Joback Method
cpg	1520.77	J/mol×K	1089.75	Joback Method
cpg	1554.50	J/mol×K	1127.10	Joback Method
cpg	1589.59	J/mol×K	1164.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368375&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

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