5«beta»-Cholestan-3«alpha»-ol, pentafluoropropionate

Inchi: InChI=1S/C30H47F5O2/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(37-26(36)29(
InchiKey: IPXMWSYJBPUDBR-UHFFFAOYSA-N
Formula: C30H47F5O2
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4CC(OC(=O)C(F)(F)C(F)(F)F)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 534.68

Physical Properties

Property code	Value	Unit	Source
gf	-864.77	kJ/mol	Joback Method
hf	-1706.42	kJ/mol	Joback Method
hfus	43.50	kJ/mol	Joback Method
hvap	81.05	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	9.217		Crippen Method
mcvol	406.410	ml/mol	McGowan Method
pc	763.10	kPa	Joback Method
rinpol	2901.40		NIST Webbook
tb	981.21	K	Joback Method
tc	1202.37	K	Joback Method
tf	562.81	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1566.90	J/mol×K	981.21	Joback Method
cpg	1598.74	J/mol×K	1018.07	Joback Method
cpg	1631.17	J/mol×K	1054.93	Joback Method
cpg	1664.52	J/mol×K	1091.79	Joback Method
cpg	1699.16	J/mol×K	1128.65	Joback Method
cpg	1735.45	J/mol×K	1165.51	Joback Method
cpg	1773.74	J/mol×K	1202.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352230&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