Cholesterol, pentafluoropropionate

Inchi: InChI=1S/C30H45F5O2/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(37-26(36)29(
InchiKey: BBOBVTCCIPFEPH-UHFFFAOYSA-N
Formula: C30H45F5O2
SMILES: CC(C)CCCC(C)C1CCC2C3CC=C4CC(OC(=O)C(F)(F)C(F)(F)F)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 532.67

Physical Properties

Property code	Value	Unit	Source
gf	-836.73	kJ/mol	Joback Method
hf	-1639.77	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	82.31	kJ/mol	Joback Method
log10ws	-9.83		Crippen Method
logp	9.137		Crippen Method
mcvol	402.110	ml/mol	McGowan Method
pc	786.39	kPa	Joback Method
rinpol	2960.60		NIST Webbook
rinpol	2960.60		NIST Webbook
tb	990.02	K	Joback Method
tc	1213.14	K	Joback Method
tf	580.33	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1533.66	J/mol×K	990.02	Joback Method
cpg	1565.26	J/mol×K	1027.21	Joback Method
cpg	1597.68	J/mol×K	1064.39	Joback Method
cpg	1631.27	J/mol×K	1101.58	Joback Method
cpg	1666.40	J/mol×K	1138.76	Joback Method
cpg	1703.44	J/mol×K	1175.95	Joback Method
cpg	1742.76	J/mol×K	1213.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352225&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