5«beta»-Pregnane-3«alpha»,20«alpha»-diol, bis(pentafluoropropionate)

Inchi: InChI=1S/C27H34F10O4/c1-13(40-20(38)24(28,29)26(32,33)34)17-6-7-18-16-5-4-14-12-

InchiKey: VEMXZGRZAVUCLD-UHFFFAOYSA-N

Formula: C27H34F10O4

SMILES: CC(OC(=O)C(F)(F)C(F)(F)F)C1CCC2C3CCC4CC(OC(=O)C(F)(F)C(F)(F)F)CCC4(C)C3C

Mol. weight [g/mol]: 612.54

Physical Properties

Property code	Value	Unit	Source
gf	-2089.88	kJ/mol	Joback Method
hf	-2882.07	kJ/mol	Joback Method
hfus	42.61	kJ/mol	Joback Method
hvap	77.24	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	7.884		Crippen Method
mcvol	380.430	ml/mol	McGowan Method
pc	825.26	kPa	Joback Method
rinpol	2485.70		NIST Webbook
tb	979.19	K	Joback Method
tc	1198.84	K	Joback Method
tf	623.95	K	Joback Method
vc	1.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1458.03	J/mol×K	979.19	Joback Method
cpg	1485.51	J/mol×K	1015.80	Joback Method
cpg	1513.79	J/mol×K	1052.41	Joback Method
cpg	1543.23	J/mol×K	1089.01	Joback Method
cpg	1574.20	J/mol×K	1125.62	Joback Method
cpg	1607.08	J/mol×K	1162.23	Joback Method
cpg	1642.23	J/mol×K	1198.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352387&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