6Alpha-fluoro-17alpha-hydroxy-16alpha-methylpr

Inchi: InChI=1S/C22H29FO3/c1-12-9-17-15-11-19(23)18-10-14(25)5-7-20(18,3)16(15)6-8-21(1
InchiKey: FBZFPANTIRWUKU-UHFFFAOYSA-N
Formula: C22H29FO3
SMILES: CC(=O)C1(O)C(C)CC2C3CC(F)C4=CC(=O)C=CC4(C)C3CCC21C
Mol. weight [g/mol]: 360.46
CAS: 5072-33-3

Physical Properties

Property code	Value	Unit	Source
gf	-263.30	kJ/mol	Joback Method
hf	-767.18	kJ/mol	Joback Method
hfus	30.50	kJ/mol	Joback Method
hvap	88.49	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.808		Crippen Method
mcvol	279.580	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
tb	949.55	K	Joback Method
tc	1184.09	K	Joback Method
tf	640.20	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.67	J/mol×K	949.55	Joback Method
cpg	1070.18	J/mol×K	988.64	Joback Method
cpg	1101.34	J/mol×K	1027.73	Joback Method
cpg	1134.57	J/mol×K	1066.82	Joback Method
cpg	1170.28	J/mol×K	1105.91	Joback Method
cpg	1208.88	J/mol×K	1145.00	Joback Method
cpg	1250.79	J/mol×K	1184.09	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5072333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume