

5-Pregnen-3-«beta»,20-«beta»-diol, HFB

Inchi:	InChI=1S/C29H32F14O4/c1-13(46-20(44)24(30,31)26(34,35)28(38,39)40)17-6-7-18-16-5
InchiKey:	XNCNNHDGAQVERN-JHLVREFVSA-N
Formula:	C29H32F14O4
SMILES:	CC(OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C1CCC2C3CC=C4CC(OC(=O)C(F)(F)C(F)(F)C(F)(F)
Mol. weight [g/mol]:	710.54

Physical Properties

Property code	Value	Unit	Source
gf	-2818.56	kJ/mol	Joback Method
hf	-3658.64	kJ/mol	Joback Method
hfus	45.04	kJ/mol	Joback Method
hvap	77.09	kJ/mol	Joback Method
log10ws	-10.47		Crippen Method
logp	9.075		Crippen Method
mcvol	411.390	ml/mol	McGowan Method
pc	706.96	kPa	Joback Method
rinpole	2593.00		NIST Webbook
rinpole	2599.00		NIST Webbook
tb	1024.38	K	Joback Method
tc	1258.51	K	Joback Method
tf	671.21	K	Joback Method
vc	1.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.64	J/molxK	1024.38	Joback Method
cpg	1616.66	J/molxK	1063.40	Joback Method
cpg	1649.54	J/molxK	1102.42	Joback Method
cpg	1684.80	J/molxK	1141.44	Joback Method
cpg	1722.97	J/molxK	1180.46	Joback Method
cpg	1764.55	J/molxK	1219.48	Joback Method
cpg	1810.07	J/molxK	1258.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R385332&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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