5-«alpha»-Pregnan-3-«alpha»,20-«alpha»-diol, HFB

Inchi: InChI=1S/C29H34F14O4/c1-13(46-20(44)24(30,31)26(34,35)28(38,39)40)17-6-7-18-16-5

InchiKey: KPANXDBYARJMLI-GBOBYPTESA-N

Formula: C29H34F14O4

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

Mol. weight [g/mol]: 712.56

Physical Properties

Property code	Value	Unit	Source
gf	-2846.60	kJ/mol	Joback Method
hf	-3725.29	kJ/mol	Joback Method
hfus	45.28	kJ/mol	Joback Method
hvap	75.83	kJ/mol	Joback Method
log10ws	-10.38		Crippen Method
logp	9.155		Crippen Method
mcvol	415.690	ml/mol	McGowan Method
pc	687.09	kPa	Joback Method
rinpol	2552.00		NIST Webbook
rinpol	2548.00		NIST Webbook
rinpol	2552.00		NIST Webbook
tb	1015.57	K	Joback Method
tc	1247.63	K	Joback Method
tf	653.69	K	Joback Method
vc	1.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1620.11	J/mol×K	1015.57	Joback Method
cpg	1651.06	J/mol×K	1054.25	Joback Method
cpg	1683.58	J/mol×K	1092.92	Joback Method
cpg	1718.17	J/mol×K	1131.60	Joback Method
cpg	1755.33	J/mol×K	1170.28	Joback Method
cpg	1795.57	J/mol×K	1208.96	Joback Method
cpg	1839.38	J/mol×K	1247.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R384948&Units=SI

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

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