5-«alpha»-Androstan-3-«beta»,16-«alpha»-diol, HFB

Inchi: InChI=1S/C27H30F14O4/c1-20-7-6-16-15(17(20)10-14(11-20)45-19(43)23(30,31)25(34,3

InchiKey: UVWRFIUMLDHHGH-SPZQWNDZSA-N

Formula: C27H30F14O4

SMILES: CC12CCC3C(CCC4CC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CCC43C)C1CC(OC(=O)C(F)(F)

Mol. weight [g/mol]: 684.50

Physical Properties

Property code	Value	Unit	Source
gf	-2861.00	kJ/mol	Joback Method
hf	-3678.73	kJ/mol	Joback Method
hfus	43.62	kJ/mol	Joback Method
hvap	71.77	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	8.519		Crippen Method
mcvol	387.510	ml/mol	McGowan Method
pc	758.49	kPa	Joback Method
rinpol	2444.00		NIST Webbook
rinpol	2444.00		NIST Webbook
rinpol	2430.00		NIST Webbook
tb	970.25	K	Joback Method
tc	1188.59	K	Joback Method
tf	646.15	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.73	J/mol×K	970.25	Joback Method
cpg	1509.14	J/mol×K	1006.64	Joback Method
cpg	1536.50	J/mol×K	1043.03	Joback Method
cpg	1565.23	J/mol×K	1079.42	Joback Method
cpg	1595.73	J/mol×K	1115.81	Joback Method
cpg	1628.42	J/mol×K	1152.20	Joback Method
cpg	1663.70	J/mol×K	1188.59	Joback Method

Sources

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=R384795&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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