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

Inchi: InChI=1S/C25H34F6O4/c1-13(34-20(32)24(26,27)28)17-6-7-18-16-5-4-14-12-15(35-21(3

InchiKey: ZYWWYWQPOLCWDY-UHFFFAOYSA-N

Formula: C25H34F6O4

SMILES: CC(OC(=O)C(F)(F)F)C1CCC2C3CCC4CC(OC(=O)C(F)(F)F)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 512.53

Physical Properties

Property code	Value	Unit	Source
gf	-1333.16	kJ/mol	Joback Method
hf	-2038.85	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.613		Crippen Method
mcvol	345.170	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
rinpol	2508.70		NIST Webbook
rinpol	2508.70		NIST Webbook
tb	942.81	K	Joback Method
tc	1159.83	K	Joback Method
tf	594.21	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1297.92	J/mol×K	942.81	Joback Method
cpg	1323.94	J/mol×K	978.98	Joback Method
cpg	1350.26	J/mol×K	1015.15	Joback Method
cpg	1377.20	J/mol×K	1051.32	Joback Method
cpg	1405.06	J/mol×K	1087.49	Joback Method
cpg	1434.12	J/mol×K	1123.66	Joback Method
cpg	1464.71	J/mol×K	1159.83	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=U352388&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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