

5-Pregnen-3-«beta»,20-«alpha»-diol, TFA

Inchi:	InChI=1S/C25H32F6O4/c1-13(34-20(32)24(26,27)28)17-6-7-18-16-5-4-14-12-15(35-21(3
InchiKey:	CEUTXEHQJLYLFE-ZZNMDPQCSA-N
Formula:	C25H32F6O4
SMILES:	CC(OC(=O)C(F)(F)F)C1CCC2C3CC=C4CC(OC(=O)C(F)(F)F)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	510.51

Physical Properties

Property code	Value	Unit	Source
gf	-1305.12	kJ/mol	Joback Method
hf	-1972.20	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	79.91	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	6.534		Crippen Method
mcvol	340.870	ml/mol	McGowan Method
pc	1045.30	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
rinpol	2529.00		NIST Webbook
rinpol	2535.00		NIST Webbook
tb	951.62	K	Joback Method
tc	1170.61	K	Joback Method
tf	611.73	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1264.21	J/molxK	951.62	Joback Method
cpg	1289.77	J/molxK	988.12	Joback Method
cpg	1315.84	J/molxK	1024.62	Joback Method
cpg	1342.73	J/molxK	1061.12	Joback Method
cpg	1370.78	J/molxK	1097.61	Joback Method
cpg	1400.27	J/molxK	1134.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R385327&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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