

5-Pregnen-3«beta»-ol-20-one, trifluoroacetate

Inchi:	InChI=1S/C23H31F3O3/c1-13(27)17-6-7-18-16-5-4-14-12-15(29-20(28)23(24,25)26)8-10
InchiKey:	XMFYUFNYYIKKQW-UHFFFAOYSA-N
Formula:	C23H31F3O3
SMILES:	CC(=O)C1CCC2C3CC=C4CC(OC(=O)C(F)(F)F)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	412.49

Physical Properties

Property code	Value	Unit	Source
gf	-632.93	kJ/mol	Joback Method
hf	-1196.34	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	77.18	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.628		Crippen Method
mcvol	301.510	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
tb	889.30	K	Joback Method
tc	1113.79	K	Joback Method
tf	577.77	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.05	J/molxK	889.30	Joback Method
cpg	1103.88	J/molxK	926.71	Joback Method
cpg	1128.87	J/molxK	964.13	Joback Method
cpg	1154.35	J/molxK	1001.54	Joback Method
cpg	1180.62	J/molxK	1038.96	Joback Method
cpg	1208.03	J/molxK	1076.37	Joback Method
cpg	1236.87	J/molxK	1113.79	Joback Method

Sources

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=U352614&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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