1,3,5(10)-Oestratrien-17«alpha»-ol, TFA

Inchi: InChI=1S/C20H23F3O2/c1-19-11-10-14-13-5-3-2-4-12(13)6-7-15(14)16(19)8-9-17(19)25
InchiKey: HOAPZVGQTWGAQC-YUAHOQAQSA-N
Formula: C20H23F3O2
SMILES: CC12CCC3c4ccccc4CCC3C1CCC2OC(=O)C(F)(F)F
Mol. weight [g/mol]: 352.39

Physical Properties

Property code	Value	Unit	Source
gf	-458.07	kJ/mol	Joback Method
hf	-892.31	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	66.78	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.017		Crippen Method
mcvol	249.070	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	2177.00		NIST Webbook
rinpol	2145.00		NIST Webbook
tb	779.19	K	Joback Method
tc	1002.66	K	Joback Method
tf	492.65	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.41	J/mol×K	779.19	Joback Method
cpg	832.53	J/mol×K	816.43	Joback Method
cpg	851.77	J/mol×K	853.68	Joback Method
cpg	870.36	J/mol×K	890.92	Joback Method
cpg	888.52	J/mol×K	928.17	Joback Method
cpg	906.49	J/mol×K	965.41	Joback Method
cpg	924.49	J/mol×K	1002.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R523698&Units=SI
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

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