1,3,5(10)-Oestratrien-3-ol, TFA

Inchi: InChI=1S/C20H23F3O2/c1-19-9-2-3-17(19)16-6-4-12-11-13(25-18(24)20(21,22)23)5-7-1
InchiKey: QCQBIIWTQYCSMP-IMBTUZDBSA-N
Formula: C20H23F3O2
SMILES: CC12CCCC1C1CCc3cc(OC(=O)C(F)(F)F)ccc3C1CC2
Mol. weight [g/mol]: 352.39

Physical Properties

Property code	Value	Unit	Source
gf	-459.99	kJ/mol	Joback Method
hf	-883.44	kJ/mol	Joback Method
hfus	30.41	kJ/mol	Joback Method
hvap	67.75	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.401		Crippen Method
mcvol	249.070	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2146.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	788.84	K	Joback Method
tc	1013.07	K	Joback Method
tf	509.41	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.91	J/mol×K	788.84	Joback Method
cpg	828.56	J/mol×K	826.21	Joback Method
cpg	847.43	J/mol×K	863.58	Joback Method
cpg	865.77	J/mol×K	900.95	Joback Method
cpg	883.80	J/mol×K	938.33	Joback Method
cpg	901.76	J/mol×K	975.70	Joback Method
cpg	919.86	J/mol×K	1013.07	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=R523787&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume