Oestrone, 6-dehydro, TFA

Inchi: InChI=1S/C20H19F3O3/c1-19-9-8-14-13-5-3-12(26-18(25)20(21,22)23)10-11(13)2-4-15(
InchiKey: YJARQWPASKZKEO-YIOZNXECSA-N
Formula: C20H19F3O3
SMILES: CC12CCC3c4ccc(OC(=O)C(F)(F)F)cc4C=CC3C1CCC2=O
Mol. weight [g/mol]: 364.36

Physical Properties

Property code	Value	Unit	Source
gf	-552.62	kJ/mol	Joback Method
hf	-963.36	kJ/mol	Joback Method
hfus	31.14	kJ/mol	Joback Method
hvap	72.28	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.660		Crippen Method
mcvol	246.340	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2417.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	855.82	K	Joback Method
tc	1091.29	K	Joback Method
tf	578.39	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.65	J/mol×K	855.82	Joback Method
cpg	834.01	J/mol×K	895.07	Joback Method
cpg	851.88	J/mol×K	934.31	Joback Method
cpg	869.50	J/mol×K	973.56	Joback Method
cpg	887.07	J/mol×K	1012.80	Joback Method
cpg	904.84	J/mol×K	1052.05	Joback Method
cpg	923.04	J/mol×K	1091.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R524057&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