Estrone, TFA

Inchi: InChI=1S/C20H21F3O3/c1-19-9-8-14-13-5-3-12(26-18(25)20(21,22)23)10-11(13)2-4-15(
InchiKey: UAPVNSRFPMGHBC-ZEPBGEJQSA-N
Formula: C20H21F3O3
SMILES: CC12CCC3c4ccc(OC(=O)C(F)(F)F)cc4CCC3C1CCC2=O
Mol. weight [g/mol]: 366.37

Physical Properties

Property code	Value	Unit	Source
gf	-582.58	kJ/mol	Joback Method
hf	-1021.14	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	71.99	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.579		Crippen Method
mcvol	250.640	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	2392.00		NIST Webbook
tb	856.66	K	Joback Method
tc	1090.57	K	Joback Method
tf	577.63	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.26	J/mol×K	856.66	Joback Method
cpg	863.43	J/mol×K	895.65	Joback Method
cpg	882.05	J/mol×K	934.63	Joback Method
cpg	900.33	J/mol×K	973.62	Joback Method
cpg	918.51	J/mol×K	1012.60	Joback Method
cpg	936.79	J/mol×K	1051.59	Joback Method
cpg	955.41	J/mol×K	1090.57	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R293877&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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