17«beta»-Oestradiol, 3-methoxy, TFA

Inchi: InChI=1S/C21H25F3O3/c1-20-10-9-15-14-6-4-13(26-2)11-12(14)3-5-16(15)17(20)7-8-18
InchiKey: RBZLYLXZTKIMFG-AUFNPSFISA-N
Formula: C21H25F3O3
SMILES: COc1ccc2c(c1)CCC1C2CCC2(C)C(OC(=O)C(F)(F)F)CCC12
Mol. weight [g/mol]: 382.42

Physical Properties

Property code	Value	Unit	Source
gf	-564.28	kJ/mol	Joback Method
hf	-1056.64	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.025		Crippen Method
mcvol	269.030	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2422.00		NIST Webbook
tb	829.47	K	Joback Method
tc	1049.30	K	Joback Method
tf	538.67	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.66	J/mol×K	829.47	Joback Method
cpg	921.65	J/mol×K	866.11	Joback Method
cpg	940.94	J/mol×K	902.75	Joback Method
cpg	959.74	J/mol×K	939.39	Joback Method
cpg	978.22	J/mol×K	976.02	Joback Method
cpg	996.60	J/mol×K	1012.66	Joback Method
cpg	1015.06	J/mol×K	1049.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R523905&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

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