trans-Dehydroandrosterone, trifluoroacetate

Inchi: InChI=1S/C21H27F3O3/c1-19-9-7-13(27-18(26)21(22,23)24)11-12(19)3-4-14-15-5-6-17(
InchiKey: DDDJCSCTQYHRFY-UHFFFAOYSA-N
Formula: C21H27F3O3
SMILES: CC12CCC3C(CC=C4CC(OC(=O)C(F)(F)F)CCC43C)C1CCC2=O
Mol. weight [g/mol]: 384.43

Physical Properties

Property code	Value	Unit	Source
gf	-635.73	kJ/mol	Joback Method
hf	-1159.84	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	70.54	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.992		Crippen Method
mcvol	273.330	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	2461.40		NIST Webbook
tb	862.16	K	Joback Method
tc	1094.91	K	Joback Method
tf	577.76	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.33	J/mol×K	862.16	Joback Method
cpg	991.42	J/mol×K	900.95	Joback Method
cpg	1015.48	J/mol×K	939.74	Joback Method
cpg	1039.83	J/mol×K	978.53	Joback Method
cpg	1064.79	J/mol×K	1017.32	Joback Method
cpg	1090.69	J/mol×K	1056.12	Joback Method
cpg	1117.84	J/mol×K	1094.91	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=U352252&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