Androsterone, trifluoroacetate

Inchi: InChI=1S/C21H29F3O3/c1-19-9-7-13(27-18(26)21(22,23)24)11-12(19)3-4-14-15-5-6-17(
InchiKey: NTPCFTHVUCOBOX-UHFFFAOYSA-N
Formula: C21H29F3O3
SMILES: CC12CCC3C(CCC4CC(OC(=O)C(F)(F)F)CCC43C)C1CCC2=O
Mol. weight [g/mol]: 386.45

Physical Properties

Property code	Value	Unit	Source
gf	-663.77	kJ/mol	Joback Method
hf	-1226.49	kJ/mol	Joback Method
hfus	26.93	kJ/mol	Joback Method
hvap	69.28	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.072		Crippen Method
mcvol	277.630	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2424.40		NIST Webbook
tb	853.35	K	Joback Method
tc	1083.86	K	Joback Method
tf	560.24	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.23	J/mol×K	853.35	Joback Method
cpg	1024.27	J/mol×K	891.77	Joback Method
cpg	1049.07	J/mol×K	930.19	Joback Method
cpg	1073.95	J/mol×K	968.60	Joback Method
cpg	1099.21	J/mol×K	1007.02	Joback Method
cpg	1125.16	J/mol×K	1045.44	Joback Method
cpg	1152.12	J/mol×K	1083.86	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=U352224&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