trans-Dehydroandrosterone, pentafluoropropionate

Inchi: InChI=1S/C22H27F5O3/c1-19-9-7-13(30-18(29)21(23,24)22(25,26)27)11-12(19)3-4-14-1

InchiKey: WQVZUVYAIXHPIW-UHFFFAOYSA-N

Formula: C22H27F5O3

SMILES: CC12CCC3C(CC=C4CC(OC(=O)C(F)(F)C(F)(F)F)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 434.44

Physical Properties

Property code	Value	Unit	Source
gf	-1014.09	kJ/mol	Joback Method
hf	-1581.45	kJ/mol	Joback Method
hfus	28.02	kJ/mol	Joback Method
hvap	69.84	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.628		Crippen Method
mcvol	290.960	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2454.20		NIST Webbook
tb	880.35	K	Joback Method
tc	1105.27	K	Joback Method
tf	592.63	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.69	J/mol×K	880.35	Joback Method
cpg	1068.26	J/mol×K	917.84	Joback Method
cpg	1091.94	J/mol×K	955.32	Joback Method
cpg	1116.05	J/mol×K	992.81	Joback Method
cpg	1140.91	J/mol×K	1030.30	Joback Method
cpg	1166.83	J/mol×K	1067.79	Joback Method
cpg	1194.15	J/mol×K	1105.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352251&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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