trans-Dehydroandrosterone, heptafluorobutyrate

Inchi: InChI=1S/C23H27F7O3/c1-19-9-7-13(33-18(32)21(24,25)22(26,27)23(28,29)30)11-12(19

InchiKey: ZSZXVWUIMGNJSD-UHFFFAOYSA-N

Formula: C23H27F7O3

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

Mol. weight [g/mol]: 484.45

Physical Properties

Property code	Value	Unit	Source
gf	-1392.45	kJ/mol	Joback Method
hf	-2003.06	kJ/mol	Joback Method
hfus	29.36	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.263		Crippen Method
mcvol	308.590	ml/mol	McGowan Method
pc	1178.47	kPa	Joback Method
rinpol	2489.10		NIST Webbook
tb	898.54	K	Joback Method
tc	1117.72	K	Joback Method
tf	607.50	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1122.35	J/mol×K	898.54	Joback Method
cpg	1145.66	J/mol×K	935.07	Joback Method
cpg	1169.24	J/mol×K	971.60	Joback Method
cpg	1193.40	J/mol×K	1008.13	Joback Method
cpg	1218.47	J/mol×K	1044.66	Joback Method
cpg	1244.77	J/mol×K	1081.19	Joback Method
cpg	1272.64	J/mol×K	1117.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352250&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

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