17-(2,4-Dinitrophenylhydrazono)-5beta-androstan

Inchi: InChI=1S/C25H34N4O5/c1-24-11-9-17(30)13-15(24)3-5-18-19-6-8-23(25(19,2)12-10-20(
InchiKey: FTLREWFXBTYMQV-SLEBQGDGSA-N
Formula: C25H34N4O5
SMILES: CC12CCC3C(CCC4CC(O)CCC43C)C1CCC2=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 470.56
CAS: 4589-93-9

Physical Properties

Property code	Value	Unit	Source
hf	-195.13	kJ/mol	Joback Method
hvap	132.57	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	5.675		Crippen Method
mcvol	352.280	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
tb	1368.01	K	Joback Method
tc	1674.85	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4589939&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

hf: Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature