Androstane-3,17-dione, (5alpha), 2,2,4,4,16,16-hexadeuterio-

Inchi: InChI=1S/C19H28O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14

InchiKey: RAJWOBJTTGJROA-FCLGVVOLSA-N

Formula: C19H22D6O2

SMILES: CC12CCC3C(CCC4CC(=O)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 294.46

Physical Properties

Property code	Value	Unit	Source
gf	20.02	kJ/mol	Joback Method
hf	-460.69	kJ/mol	Joback Method
hfus	15.57	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.167		Crippen Method
mcvol	238.270	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
tb	809.21	K	Joback Method
tc	1073.00	K	Joback Method
tf	533.81	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.08	J/mol×K	809.21	Joback Method
cpg	862.01	J/mol×K	853.18	Joback Method
cpg	889.40	J/mol×K	897.14	Joback Method
cpg	916.66	J/mol×K	941.11	Joback Method
cpg	944.17	J/mol×K	985.07	Joback Method
cpg	972.33	J/mol×K	1029.04	Joback Method
cpg	1001.55	J/mol×K	1073.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009861&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume