

Androsta-4-ene-3,17-dione, 1alpha-deuterio-

Inchi: InChI=1S/C19H26O2/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: AEMFNILZOJDQLW-QOWOAITPSA-N
Formula: C19H25DO2
SMILES: CC12CCC3C(CCC4=CC(=O)CCC43C)C1CCC2=O
Mol. weight [g/mol]: 287.41

Physical Properties

Property code	Value	Unit	Source
gf	48.06	kJ/mol	Joback Method
hf	-394.04	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	65.24	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.087		Crippen Method
mcvol	233.970	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
tb	818.02	K	Joback Method
tc	1084.47	K	Joback Method
tf	551.33	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.48	J/molxK	818.02	Joback Method
cpg	830.12	J/molxK	862.43	Joback Method
cpg	856.47	J/molxK	906.84	Joback Method
cpg	882.94	J/molxK	951.24	Joback Method
cpg	909.95	J/molxK	995.65	Joback Method
cpg	937.91	J/molxK	1040.06	Joback Method
cpg	967.22	J/molxK	1084.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009860&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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