

Androst-4-ene-3,11,17-trione

Other names:	11-Oxy-4-androstenedione 4-Androsten-3,11,17-trione Adrenosterone Reichstein's substance g
Inchi:	InChI=1S/C19H24O3/c1-18-8-7-12(20)9-11(18)3-4-13-14-5-6-16(22)19(14,2)10-15(21)17
InchiKey:	RZRPTBIGEANTGU-UHFFFAOYSA-N
Formula:	C19H24O3
SMILES:	CC12CC(=O)C3C(CCC4=CC(=O)CCC43C)C1CCC2=O
Mol. weight [g/mol]:	300.39
CAS:	382-45-6

Physical Properties

Property code	Value	Unit	Source
gf	-74.53	kJ/mol	Joback Method
hf	-531.74	kJ/mol	Joback Method
hfus	14.84	kJ/mol	Joback Method
hvap	69.48	kJ/mol	Joback Method
log10ws	-3.48		Aqueous Solubility Prediction Method
log10ws	-3.48		Estimated Solubility Method
logp	3.266		Crippen Method
mvol	235.540	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	2801.30		NIST Webbook
rinpol	2801.30		NIST Webbook
tb	885.84	K	Joback Method
tc	1160.74	K	Joback Method
tf	619.55	K	Joback Method
vc	0.889	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	844.28	J/molxK	885.84	Joback Method
cpg	871.27	J/molxK	931.66	Joback Method
cpg	898.32	J/molxK	977.47	Joback Method
cpg	925.84	J/molxK	1023.29	Joback Method
cpg	954.21	J/molxK	1069.11	Joback Method
cpg	983.81	J/molxK	1114.92	Joback Method
cpg	1015.04	J/molxK	1160.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C382456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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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