Calusterone

Other names:	Androst-4-en-3-one, 17-hydroxy-7,17-dimethyl-, (7«beta»,17«beta»)- Androst-4-en-3-one, 17«beta»-hydroxy-7«beta»,17-dimethyl- Calusteron Methosarb U-22,550 7«beta»,17«alpha»-Dimethyltestosterone 7«beta»,17-Dimethyltestosterone Androst-4-en-3-one, 7«beta»,17«alpha»-dimethyl-17«beta»-hydroxy- CLS Dimethyltestosterone U 22550 17«beta»-Hydroxy-7«beta»,17«alpha»-dimethylandrost-4-ene-3-one 17«beta»-Hydroxy-7«beta»,17-dimethylandrost-4-en-3-one NSC-88536 Testosterone, 7«beta»,17-dimethyl-
Inchi:	InChI=1S/C21H32O2/c1-13-11-14-12-15(22)5-8-19(14,2)16-6-9-20(3)17(18(13)16)7-10-2
InchiKey:	IVFYLRMMHVYGJH-UHFFFAOYSA-N
Formula:	C21H32O2
SMILES:	CC1CC2=CC(=O)CCC2(C)C2CCC3(C)C(CCC3(C)O)C12
Mol. weight [g/mol]:	316.48
CAS:	17021-26-0

Physical Properties

Property code	Value	Unit	Source
gf	29.76	kJ/mol	Joback Method
hf	-475.29	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.515		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	879.04	K	Joback Method
tc	1115.52	K	Joback Method
tf	581.89	K	Joback Method

vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.45	J/mol×K	879.04	Joback Method
cpg	993.76	J/mol×K	918.45	Joback Method
cpg	1023.08	J/mol×K	957.87	Joback Method
cpg	1053.82	J/mol×K	997.28	Joback Method
cpg	1086.44	J/mol×K	1036.69	Joback Method
cpg	1121.35	J/mol×K	1076.11	Joback Method
cpg	1158.99	J/mol×K	1115.52	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17021260&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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