

Epitestosterone, octanoate

Inchi:	InChI=1S/C27H42O3/c1-4-5-6-7-8-9-25(29)30-24-13-12-22-21-11-10-19-18-20(28)14-16
InchiKey:	KCQOWSKVHVGCCF-UHFFFAOYSA-N
Formula:	C27H42O3
SMILES:	CCCCCCCC(=O)OC1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	414.62

Physical Properties

Property code	Value	Unit	Source
gf	-3.62	kJ/mol	Joback Method
hf	-686.60	kJ/mol	Joback Method
hfus	40.40	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	6.791		Crippen Method
mvol	352.560	ml/mol	McGowan Method
pc	1082.78	kPa	Joback Method
rinpol	2755.00		NIST Webbook
rinpol	2755.00		NIST Webbook
tb	1004.86	K	Joback Method
tc	1240.92	K	Joback Method
tf	641.19	K	Joback Method
vc	1.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.26	J/molxK	1004.86	Joback Method
cpg	1375.64	J/molxK	1044.20	Joback Method
cpg	1407.71	J/molxK	1083.55	Joback Method
cpg	1440.80	J/molxK	1122.89	Joback Method
cpg	1475.24	J/molxK	1162.24	Joback Method
cpg	1511.37	J/molxK	1201.58	Joback Method
cpg	1549.50	J/molxK	1240.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U368369&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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