

3-(Pronanoyloxy)-estra-1,3,5(10)-trien-17-one

Other names:	Estrone, propionate 3-(1-Oxypropoxy)-estra-1,3,5(10)-trien-17-one
Inchi:	InChI=1S/C21H26O3/c1-3-20(23)24-14-5-7-15-13(12-14)4-6-17-16(15)10-11-21(2)18(17)
InchiKey:	ROFBJLDRYQWJFI-UHFFFAOYSA-N
Formula:	C21H26O3
SMILES:	CCC(=O)Oc1ccc2c(c1)CCC1C2CCC2(C)C(=O)CCC12
Mol. weight [g/mol]:	326.43
CAS:	975-64-4

Physical Properties

Property code	Value	Unit	Source
gf	7.43	kJ/mol	Joback Method
hf	-444.70	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	77.97	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.427		Crippen Method
mcvol	259.420	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2442.00		NIST Webbook
tb	884.96	K	Joback Method
tc	1130.24	K	Joback Method
tf	584.71	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.44	J/mol×K	1089.36	Joback Method
cpg	882.21	J/mol×K	884.96	Joback Method
cpg	903.76	J/mol×K	925.84	Joback Method
cpg	924.73	J/mol×K	966.72	Joback Method
cpg	945.36	J/mol×K	1007.60	Joback Method
cpg	965.85	J/mol×K	1048.48	Joback Method

cpg	1007.35	J/mol×K	1130.24	Joback Method
hfust	23.00	kJ/mol	409.00	NIST Webbook

Sources

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=C975644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
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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