Estrone, benzoate

Other names:	Benzoate d'oestrone
	3-(Benzoyloxy)estra-1,3,5(10)-trien-17-one
	3-Hydroxyestra-1,3,5(10)-trien-17-one benzoate
	Ketohydroxyestrin benzoate
	Ketohydroxyoestrin benzoate
	Oestronbenzoat
	Estra-1,3,5(10)-trien-17-one, 3-(benzoyloxy)-
	Estrone 3-benzoate
Inchi:	InChI=1S/C25H26O3/c1-25-14-13-20-19-10-8-18(28-24(27)16-5-3-2-4-6-16)15-17(19)7-9
InchiKey:	HKUKRSLIEVXDMS-UHFFFAOYSA-N
Formula:	C25H26O3
SMILES:	CC12CCC3c4ccc(OC(=O)c5ccccc5)cc4CCC3C1CCC2=O
Mol. weight [g/mol]:	374.47
CAS:	2393-53-5

Physical Properties

Property code	Value	Unit	Source
gf	153.52	kJ/mol	Joback Method
hf	-290.73	kJ/mol	Joback Method
hfus	35.09	kJ/mol	Joback Method
hvap	89.15	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.331		Crippen Method
mcvol	292.020	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
tb	1003.16	K	Joback Method
tc	1268.71	K	Joback Method
tf	656.21	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.04	J/mol×K	1003.16	Joback Method

cpg	1054.18	J/mol×K	1047.42	Joback Method
cpg	1077.36	J/mol×K	1091.68	Joback Method
cpg	1100.88	J/mol×K	1135.94	Joback Method
cpg	1125.08	J/mol×K	1180.19	Joback Method
cpg	1150.28	J/mol×K	1224.45	Joback Method
cpg	1176.79	J/mol×K	1268.71	Joback Method

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=C2393535&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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