17Beta-acetoxy-2,4-dibromoestra-1,3,5(10)-trien-3

Inchi: InChI=1S/C20H24Br2O3/c1-10(23)25-17-6-5-15-12-3-4-13-14(9-16(21)19(24)18(13)22)1
InchiKey: YGDGJBWJHHTLMF-UHFFFAOYSA-N
Formula: C20H24Br2O3
SMILES: CC(=O)OC1CCC2C3CCc4c(cc(Br)c(O)c4Br)C3CCC12C
Mol. weight [g/mol]: 472.21
CAS: 95946-09-1

Physical Properties

Property code	Value	Unit	Source
gf	-21.72	kJ/mol	Joback Method
hf	-442.82	kJ/mol	Joback Method
hfus	45.62	kJ/mol	Joback Method
hvap	97.73	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	5.705		Crippen Method
mcvol	284.630	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	1007.51	K	Joback Method
tc	1271.45	K	Joback Method
tf	744.82	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.04	J/mol×K	1007.51	Joback Method
cpg	963.34	J/mol×K	1051.50	Joback Method
cpg	989.00	J/mol×K	1095.49	Joback Method
cpg	1016.45	J/mol×K	1139.48	Joback Method
cpg	1046.07	J/mol×K	1183.47	Joback Method
cpg	1078.28	J/mol×K	1227.46	Joback Method
cpg	1113.48	J/mol×K	1271.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C95946091&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume