17«alpha»-ethynylestradiol, 3-propionate

Inchi: InChI=1S/C23H28O3/c1-4-21(24)26-16-7-9-17-15(14-16)6-8-19-18(17)10-12-22(3)20(19
InchiKey: SWOKVUKTFUUZQW-UHFFFAOYSA-N
Formula: C23H28O3
SMILES: C#CC1(O)CCC2C3CCc4cc(OC(=O)CC)ccc4C3CCC21C
Mol. weight [g/mol]: 352.47

Physical Properties

Property code	Value	Unit	Source
gf	219.91	kJ/mol	Joback Method
hf	-213.71	kJ/mol	Joback Method
hfus	38.19	kJ/mol	Joback Method
hvap	93.25	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.222		Crippen Method
mcvol	283.300	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2468.00		NIST Webbook
tb	940.77	K	Joback Method
tc	1175.83	K	Joback Method
tf	666.48	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.78	J/mol×K	940.77	Joback Method
cpg	1007.52	J/mol×K	979.95	Joback Method
cpg	1033.31	J/mol×K	1019.12	Joback Method
cpg	1060.49	J/mol×K	1058.30	Joback Method
cpg	1089.41	J/mol×K	1097.48	Joback Method
cpg	1120.44	J/mol×K	1136.66	Joback Method
cpg	1153.92	J/mol×K	1175.83	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=U368388&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