17«alpha»-ethynylestradiol, 3-butyrate

Inchi: InChI=1S/C24H30O3/c1-4-6-22(25)27-17-8-10-18-16(15-17)7-9-20-19(18)11-13-23(3)21
InchiKey: FIPNBJWTSLURCK-UHFFFAOYSA-N
Formula: C24H30O3
SMILES: C#CC1(O)CCC2C3CCc4cc(OC(=O)CCC)ccc4C3CCC21C
Mol. weight [g/mol]: 366.49

Physical Properties

Property code	Value	Unit	Source
gf	228.33	kJ/mol	Joback Method
hf	-234.35	kJ/mol	Joback Method
hfus	40.78	kJ/mol	Joback Method
hvap	95.47	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	4.613		Crippen Method
mcvol	297.390	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2522.00		NIST Webbook
tb	963.65	K	Joback Method
tc	1197.65	K	Joback Method
tf	677.75	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1047.89	J/mol×K	963.65	Joback Method
cpg	1073.97	J/mol×K	1002.65	Joback Method
cpg	1101.22	J/mol×K	1041.65	Joback Method
cpg	1129.99	J/mol×K	1080.65	Joback Method
cpg	1160.66	J/mol×K	1119.65	Joback Method
cpg	1193.55	J/mol×K	1158.65	Joback Method
cpg	1229.04	J/mol×K	1197.65	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=U368389&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume