17«alpha»-ethynylestradiol, 3-acetate

Inchi: InChI=1S/C22H26O3/c1-4-22(24)12-10-20-19-7-5-15-13-16(25-14(2)23)6-8-17(15)18(19
InchiKey: WHONTIANOSNSAH-UHFFFAOYSA-N
Formula: C22H26O3
SMILES: C#CC1(O)CCC2C3CCc4cc(OC(C)=O)ccc4C3CCC21C
Mol. weight [g/mol]: 338.44

Physical Properties

Property code	Value	Unit	Source
gf	211.49	kJ/mol	Joback Method
hf	-193.07	kJ/mol	Joback Method
hfus	35.60	kJ/mol	Joback Method
hvap	91.02	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	3.832		Crippen Method
mcvol	269.210	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
tb	917.89	K	Joback Method
tc	1154.81	K	Joback Method
tf	655.21	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.00	J/mol×K	917.89	Joback Method
cpg	942.54	J/mol×K	957.38	Joback Method
cpg	966.99	J/mol×K	996.86	Joback Method
cpg	992.70	J/mol×K	1036.35	Joback Method
cpg	1020.05	J/mol×K	1075.83	Joback Method
cpg	1049.38	J/mol×K	1115.32	Joback Method
cpg	1081.05	J/mol×K	1154.81	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=U368387&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume