17«alpha»-ethynylestradiol, 3-formate

Inchi: InChI=1S/C21H24O3/c1-3-21(23)11-9-19-18-6-4-14-12-15(24-13-22)5-7-16(14)17(18)8-1
InchiKey: PJRWMJBAAOIMHI-UHFFFAOYSA-N
Formula: C21H24O3
SMILES: C#CC1(O)CCC2C3CCc4cc(OC=O)ccc4C3CCC21C
Mol. weight [g/mol]: 324.41

Physical Properties

Property code	Value	Unit	Source
gf	232.47	kJ/mol	Joback Method
hf	-145.43	kJ/mol	Joback Method
hfus	33.70	kJ/mol	Joback Method
hvap	88.77	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	3.442		Crippen Method
mcvol	255.120	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook
tb	889.80	K	Joback Method
tc	1125.71	K	Joback Method
tf	636.01	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.56	J/mol×K	889.80	Joback Method
cpg	877.50	J/mol×K	929.12	Joback Method
cpg	900.17	J/mol×K	968.44	Joback Method
cpg	923.94	J/mol×K	1007.76	Joback Method
cpg	949.15	J/mol×K	1047.08	Joback Method
cpg	976.16	J/mol×K	1086.39	Joback Method
cpg	1005.30	J/mol×K	1125.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368386&Units=SI
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

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