Hexestrol, O-acetyl-

Inchi: InChI=1S/C20H24O3/c1-4-19(15-6-10-17(22)11-7-15)20(5-2)16-8-12-18(13-9-16)23-14(3
InchiKey: POZGCPKJFGPFIS-UHFFFAOYSA-N
Formula: C20H24O3
SMILES: CCC(c1ccc(O)cc1)C(CC)c1ccc(OC(C)=O)cc1
Mol. weight [g/mol]: 312.40

Physical Properties

Property code	Value	Unit	Source
gf	-60.71	kJ/mol	Joback Method
hf	-427.21	kJ/mol	Joback Method
hfus	36.77	kJ/mol	Joback Method
hvap	86.72	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	5.005		Crippen Method
mcvol	258.450	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
tb	871.37	K	Joback Method
tc	1104.98	K	Joback Method
tf	534.40	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.86	J/mol×K	871.37	Joback Method
cpg	809.50	J/mol×K	910.31	Joback Method
cpg	824.18	J/mol×K	949.24	Joback Method
cpg	838.02	J/mol×K	988.18	Joback Method
cpg	851.13	J/mol×K	1027.11	Joback Method
cpg	863.62	J/mol×K	1066.05	Joback Method
cpg	875.61	J/mol×K	1104.98	Joback Method
dvisc	0.0001247	Pa×s	534.40	Joback Method

dvisc	0.0000497	Pa×s	590.56	Joback Method
dvisc	0.0000233	Pa×s	646.72	Joback Method
dvisc	0.0000123	Pa×s	702.88	Joback Method
dvisc	0.0000071	Pa×s	759.05	Joback Method
dvisc	0.0000045	Pa×s	815.21	Joback Method
dvisc	0.0000030	Pa×s	871.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374878&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
dvisc:	Dynamic viscosity
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