

3-Methoxy-17alpha-oxa-d-homoestra-1,3,5(10)-trien-2-one

Inchi:	InChI=1S/C19H24O3/c1-19-10-9-15-14-6-4-13(21-2)11-12(14)3-5-16(15)17(19)7-8-18(20)
InchiKey:	INHMMEWBTMZCLR-UHFFFAOYSA-N
Formula:	C19H24O3
SMILES:	COc1ccc2c(c1)CCC1C2CCC2(C)OC(=O)CCC12
Mol. weight [g/mol]:	300.39
CAS:	64945-54-6

Physical Properties

Property code	Value	Unit	Source
gf	21.29	kJ/mol	Joback Method
hf	-429.00	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.847		Crippen Method
mcvol	235.540	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
tb	816.55	K	Joback Method
tc	1069.56	K	Joback Method
tf	535.29	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.57	J/molxK	816.55	Joback Method
cpg	801.82	J/molxK	858.72	Joback Method
cpg	823.10	J/molxK	900.89	Joback Method
cpg	843.66	J/molxK	943.05	Joback Method
cpg	863.70	J/molxK	985.22	Joback Method
cpg	883.45	J/molxK	1027.39	Joback Method
cpg	903.12	J/molxK	1069.56	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=C64945546&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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