D-Homoestra-1,3,5(10)-trien-17a-one,3-methoxy-,(

Inchi: InChI=1S/C20H26O2/c1-20-10-9-17-16-7-5-15(22-2)11-13(16)3-6-18(17)19(20)8-4-14(21

InchiKey: TUNMWZWFKFYHNV-HTYYJLERSA-N

Formula: C20H26O2

SMILES: COc1ccc2c(c1)CCC1C2CCC2(C)CC(=O)CCC12

Mol. weight [g/mol]: 298.42

CAS: 1232-88-8

Physical Properties

Property code	Value	Unit	Source
gf	115.83	kJ/mol	Joback Method
hf	-317.64	kJ/mol	Joback Method
hfus	24.39	kJ/mol	Joback Method
hvap	69.17	kJ/mol	Joback Method
ie	8.17 ± 0.08	eV	NIST Webbook
log10ws	-5.17		Crippen Method
logp	4.511		Crippen Method
mcvol	243.760	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
tb	812.48	K	Joback Method
tc	1064.10	K	Joback Method
tf	519.99	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.72	J/mol×K	812.48	Joback Method
cpg	828.08	J/mol×K	854.42	Joback Method
cpg	850.43	J/mol×K	896.35	Joback Method
cpg	871.97	J/mol×K	938.29	Joback Method
cpg	892.95	J/mol×K	980.23	Joback Method
cpg	913.59	J/mol×K	1022.16	Joback Method
cpg	934.11	J/mol×K	1064.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1232888&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

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
ie:	Ionization energy
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