trans-Androsterone, methyl ether

Inchi: InChI=1S/C20H32O2/c1-19-10-8-14(22-3)12-13(19)4-5-15-16-6-7-18(21)20(16,2)11-9-17
InchiKey: OZUIPNMWFGWFOM-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: COC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	38.32	kJ/mol	Joback Method
hf	-496.19	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	64.05	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.613		Crippen Method
mcvol	256.660	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	2564.60		NIST Webbook
rinpol	2564.60		NIST Webbook
tb	782.02	K	Joback Method
tc	1027.22	K	Joback Method
tf	494.85	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.56	J/mol×K	782.02	Joback Method
cpg	913.78	J/mol×K	822.89	Joback Method
cpg	941.22	J/mol×K	863.75	Joback Method
cpg	968.20	J/mol×K	904.62	Joback Method
cpg	995.05	J/mol×K	945.49	Joback Method
cpg	1022.12	J/mol×K	986.35	Joback Method
cpg	1049.73	J/mol×K	1027.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332794&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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