

trans-Dehydroandrosterone, methyl ether

Other names:	(3«beta»)-3-Methoxyandrost-5-en-17-one
Inchi:	InChI=1S/C20H30O2/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:	FLCAHAJJOOEIKL-UHFFFAOYSA-N
Formula:	C20H30O2
SMILES:	COC1CCC2(C)C(=CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]:	302.45

Physical Properties

Property code	Value	Unit	Source
gf	66.36	kJ/mol	Joback Method
hf	-429.54	kJ/mol	Joback Method
hfus	20.67	kJ/mol	Joback Method
hvap	65.32	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.533		Crippen Method
mcvol	252.360	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2544.60		NIST Webbook
rinpol	2544.60		NIST Webbook
tb	790.83	K	Joback Method
tc	1038.60	K	Joback Method
tf	512.37	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.43	J/mol×K	790.83	Joback Method
cpg	883.31	J/mol×K	832.12	Joback Method
cpg	909.62	J/mol×K	873.42	Joback Method
cpg	935.68	J/mol×K	914.71	Joback Method
cpg	961.86	J/mol×K	956.01	Joback Method
cpg	988.50	J/mol×K	997.30	Joback Method
cpg	1015.94	J/mol×K	1038.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332997&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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