

Ethisterone

Inchi:	InChI=1S/C21H28O2/c1-4-21(23)12-9-18-16-6-5-14-13-15(22)7-10-19(14,2)17(16)8-11-2
InchiKey:	CHNXZKVNWQUJIB-XOFSEUKCSA-N
Formula:	C21H28O2
SMILES:	C#CC1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	312.45
CAS:	17554-63-1

Physical Properties

Property code	Value	Unit	Source
gf	260.54	kJ/mol	Joback Method
hf	-163.05	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	80.52	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.883		Crippen Method
mcvol	257.850	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
tb	873.83	K	Joback Method
tc	1122.27	K	Joback Method
tf	633.10	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.56	J/mol×K	873.83	Joback Method
cpg	930.26	J/mol×K	915.24	Joback Method
cpg	959.28	J/mol×K	956.64	Joback Method
cpg	990.16	J/mol×K	998.05	Joback Method
cpg	1023.41	J/mol×K	1039.46	Joback Method
cpg	1059.55	J/mol×K	1080.87	Joback Method
cpg	1099.10	J/mol×K	1122.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17554631&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
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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