

Norethisterone

Inchi:	InChI=1S/C20H26O3/c1-3-19(22)10-8-16-15-5-4-13-12-14(21)6-11-20(13,23)17(15)7-9-1
InchiKey:	GYRPICHNIDQFOD-UHFFFAOYSA-N
Formula:	C20H26O3
SMILES:	C#CC1(O)CCC2C3CCC4=CC(=O)CCC4(O)C3CCC21C
Mol. weight [g/mol]:	314.42

Physical Properties

Property code	Value	Unit	Source
gf	115.30	kJ/mol	Joback Method
hf	-294.64	kJ/mol	Joback Method
hfus	24.34	kJ/mol	Joback Method
hvap	94.97	kJ/mol	Joback Method
log10ws	-4.57		Estimated Solubility Method
log10ws	-4.57		Aqueous Solubility Prediction Method
logp	2.607		Crippen Method
mvol	249.630	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	943.13	K	Joback Method
tc	1181.17	K	Joback Method
tf	682.65	K	Joback Method
vc	0.928	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.87	J/molxK	943.13	Joback Method
cpg	945.96	J/molxK	982.80	Joback Method
cpg	976.11	J/molxK	1022.48	Joback Method
cpg	1008.77	J/molxK	1062.15	Joback Method
cpg	1044.40	J/molxK	1101.82	Joback Method
cpg	1083.45	J/molxK	1141.49	Joback Method
cpg	1126.39	J/molxK	1181.17	Joback Method

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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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