Mifepristone

Other names:	11.beta.-[p-(Dimethylamino)phenyl]-17.beta.-hydroxy-17-(1-propynyl)estra-4,9-dien-3-one 11«beta»-[p-(Dimethylamino)phenyl]-17«beta»-hydroxy-17-(1-propynyl)estra-4,9-dien-3-o 17«beta»-hydroxy-11«beta»-[4-(dimethylamino)-phenyl]-17«alpha»-(prop-1-ynyl)-estra-4, Estra-4,9-dien-3-one, (Mifepristone) 11-[4-(dimethylamino)phenyl]-17-hydroxy-17-(1-propyn-1-yl)-, Mifegyne (11«beta»,17«beta»)- RU-38486 RU-486
Inchi:	InChI=1S/C29H35NO2/c1-5-15-29(32)16-14-26-24-12-8-20-17-22(31)11-13-23(20)27(24
InchiKey:	VKHAHZOOUSRJNA-UHFFFAOYSA-N
Formula:	C29H35NO2
SMILES:	CC#CC1(O)CCC2C3CCC4=CC(=O)CCC4=C3C(c3ccc(N(C)C)cc3)CC21C
Mol. weight [g/mol]:	429.59
CAS:	84371-65-3

Physical Properties

Property code	Value	Unit	Source
gf	545.09	kJ/mol	Joback Method
hf	-15.24	kJ/mol	Joback Method
hfus	46.05	kJ/mol	Joback Method
hvap	108.68	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	5.407		Crippen Method
mcvol	352.490	ml/mol	McGowan Method
pc	1400.64	kPa	Joback Method
tb	1133.40	K	Joback Method
tc	1397.27	K	Joback Method
tf	859.94	K	Joback Method
tt	465.45	K	Measurement and Correlation of the Solubility of Mifepristone in Eight Pure and Water + Methanol Mixed Solvents at Temperatures from 273.15 to 318.15 K
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1373.91	J/mol×K	1133.40	Joback Method
cpg	1413.71	J/mol×K	1177.38	Joback Method
cpg	1456.46	J/mol×K	1221.36	Joback Method
cpg	1502.68	J/mol×K	1265.34	Joback Method
cpg	1552.88	J/mol×K	1309.32	Joback Method
cpg	1607.55	J/mol×K	1353.29	Joback Method
cpg	1667.22	J/mol×K	1397.27	Joback Method
hfust	31.70	kJ/mol	467.10	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Measurement and Correlation of the Solubility of Mifepristone in Eight Pure and Water + Methanol Mixed Solvents at Temperatures from 273.15 to 318.15 K.: https://www.doi.org/10.1021/acs.jced.8b01062

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=C84371653&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
hfust: Enthalpy of fusion at a given temperature
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

tt: Triple Point Temperature

vc: Critical Volume