Levonorgestrel

Other names: (17.alpha.)-13-ethyl-17-hydroxy-18,19-dinorpregn-4-en-20-yn-3-one
Inchi: InChI=1S/C21H28O2/c1-3-20-11-9-17-16-8-6-15(22)13-14(16)5-7-18(17)19(20)10-12-21
InchiKey: WWYNJERNGUHSAO-XUDSTZEESA-N
Formula: C21H28O2
SMILES: C#CC1(O)CCC2C3CCC4=CC(=O)CCC4C3CCC21CC
Mol. weight [g/mol]: 312.45

Physical Properties

Property code	Value	Unit	Source
hfus	29.14	kJ/mol	Joback Method
log10ws	-5.01		Cheméo Relay (1.0)
logp	3.883		Crippen Method
mcvol	257.850	ml/mol	McGowan Method
tf	446.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.16	J/mol×K	873.59	Joback Method
cpg	929.88	J/mol×K	913.83	Joback Method
cpg	954.91	J/mol×K	954.07	Joback Method
cpg	980.63	J/mol×K	994.31	Joback Method
cpg	1007.39	J/mol×K	1034.55	Joback Method
cpg	1035.55	J/mol×K	1074.80	Joback Method
cpg	1065.47	J/mol×K	1115.04	Joback Method

Sources

Solubility of megestrol acetate and levonorgestrel in supercriticalcarbon dioxide: https://www.doi.org/10.1016/j.tca.2013.07.018
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point