4-Pregnen-3-one

Inchi: InChI=1S/C21H32O/c1-4-14-6-8-18-17-7-5-15-13-16(22)9-11-21(15,3)19(17)10-12-20(14
InchiKey: AYGFEWYXKDFVIQ-MBJUYHOMSA-N
Formula: C21H32O
SMILES: CCC1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 300.48

Physical Properties

Property code	Value	Unit	Source
gf	179.78	kJ/mol	Joback Method
hf	-317.96	kJ/mol	Joback Method
hfus	22.07	kJ/mol	Joback Method
hvap	65.13	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.545		Crippen Method
mcvol	260.580	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	2531.00		NIST Webbook
tb	791.29	K	Joback Method
tc	1037.86	K	Joback Method
tf	501.41	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.99	J/mol×K	791.29	Joback Method
cpg	912.62	J/mol×K	832.39	Joback Method
cpg	939.69	J/mol×K	873.48	Joback Method
cpg	966.55	J/mol×K	914.58	Joback Method
cpg	993.58	J/mol×K	955.67	Joback Method
cpg	1021.15	J/mol×K	996.77	Joback Method
cpg	1049.63	J/mol×K	1037.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R486336&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume