

5-Pregnen-3-chloro-20-one

Inchi:	InChI=1S/C21H31ClO/c1-13(23)17-6-7-18-16-5-4-14-12-15(22)8-10-20(14,2)19(16)9-11-
InchiKey:	OIDXWRLKJLJKRZ-UHFFFAOYSA-N
Formula:	C21H31ClO
SMILES:	CC(=O)C1CCC2C3CC=C4CC(Cl)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	334.92

Physical Properties

Property code	Value	Unit	Source
gf	153.81	kJ/mol	Joback Method
hf	-328.92	kJ/mol	Joback Method
hfus	29.43	kJ/mol	Joback Method
hvap	71.71	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.762		Crippen Method
mvol	272.820	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	2388.00		NIST Webbook
rinpol	2388.00		NIST Webbook
tb	810.10	K	Joback Method
tc	1054.14	K	Joback Method
tf	508.80	K	Joback Method
vc	1.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.36	J/mol×K	810.10	Joback Method
cpg	931.60	J/mol×K	850.77	Joback Method
cpg	957.52	J/mol×K	891.45	Joback Method
cpg	983.52	J/mol×K	932.12	Joback Method
cpg	1010.00	J/mol×K	972.79	Joback Method
cpg	1037.35	J/mol×K	1013.47	Joback Method
cpg	1065.96	J/mol×K	1054.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U368374&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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