N-cyano-n-methyl-5alpha-pregnan-18-amine

Inchi: InChI=1S/C23H38N2/c1-4-17-9-11-21-19-10-8-18-7-5-6-13-22(18,2)20(19)12-14-23(17,2
InchiKey: LFUCSBAKSOGICG-UHFFFAOYSA-N
Formula: C23H38N2
SMILES: CCC1CCC2C3CCC4CCCCC4(C)C3CCC12CN(C)C#N
Mol. weight [g/mol]: 342.56
CAS: 76938-41-5

Physical Properties

Property code	Value	Unit	Source
gf	535.13	kJ/mol	Joback Method
hf	-55.78	kJ/mol	Joback Method
hfus	32.51	kJ/mol	Joback Method
hvap	76.60	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.838		Crippen Method
mcvol	302.850	ml/mol	McGowan Method
pc	1260.16	kPa	Joback Method
tb	874.94	K	Joback Method
tc	1108.80	K	Joback Method
tf	535.67	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.53	J/mol×K	874.94	Joback Method
cpg	1119.74	J/mol×K	913.92	Joback Method
cpg	1148.05	J/mol×K	952.89	Joback Method
cpg	1176.82	J/mol×K	991.87	Joback Method
cpg	1206.43	J/mol×K	1030.85	Joback Method
cpg	1237.25	J/mol×K	1069.83	Joback Method
cpg	1269.65	J/mol×K	1108.80	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=C76938415&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume