

Allopregnane

Other names:	Pregnane, (5«alpha»)- 5«alpha»-Pregnane
Inchi:	InChI=1S/C21H36/c1-4-15-9-11-18-17-10-8-16-7-5-6-13-20(16,2)19(17)12-14-21(15,18)3
InchiKey:	JWMFYGXQPXQEEM-HDOLRXQOSA-N
Formula:	C21H36
SMILES:	CCC1CCC2C3CCC4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]:	288.51
CAS:	641-85-0

Physical Properties

Property code	Value	Unit	Source
gf	274.33	kJ/mol	Joback Method
hf	-246.91	kJ/mol	Joback Method
hfus	22.80	kJ/mol	Joback Method
hvap	59.62	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	6.445		Crippen Method
mcvol	263.310	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	2175.00		NIST Webbook
rinpol	2267.00		NIST Webbook
rinpol	2175.00		NIST Webbook
tb	714.66	K	Joback Method
tc	948.64	K	Joback Method
tf	415.67	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.40	J/molxK	714.66	Joback Method
cpg	892.94	J/molxK	753.66	Joback Method
cpg	921.23	J/molxK	792.65	Joback Method
cpg	948.62	J/molxK	831.65	Joback Method

cpg	975.48	J/mol×K	870.65	Joback Method
cpg	1002.16	J/mol×K	909.64	Joback Method
cpg	1029.00	J/mol×K	948.64	Joback Method

Sources

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=C641850&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mvol:	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

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