

5«beta»-pregnane-3«alpha»,11«beta»,17«alpha»,20«beta»-pregnane

InChI: InChI=1S/C19H32O5/c20-9-17(23)19(24)6-5-13-14-3-1-10-7-11(21)2-4-12(10)18(14)16(22)1
InchiKey: KEDYQHFGKCLKUDH-QYNBOFHISA-N

Formula: C19H32O5

SMILES: OCC(O)C1(O)CCC2C3CCC4CC(O)CCC4C3C(O)CC21

Mol. weight [g/mol]: 340.45

Physical Properties

Property code	Value	Unit	Source
gf	-438.98	kJ/mol	Joback Method
hf	-1027.98	kJ/mol	Joback Method
hfus	42.98	kJ/mol	Joback Method
hvap	138.71	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	0.665		Crippen Method
mcvol	264.480	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	3088.00		NIST Webbook
rinpol	3088.00		NIST Webbook
tb	1119.78	K	Joback Method
tc	1389.72	K	Joback Method
tf	649.85	K	Joback Method
vc	0.970	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.83	J/molxK	1119.78	Joback Method
cpg	1156.27	J/molxK	1164.77	Joback Method
cpg	1183.78	J/molxK	1209.76	Joback Method
cpg	1212.73	J/molxK	1254.75	Joback Method
cpg	1243.48	J/molxK	1299.74	Joback Method
cpg	1276.40	J/molxK	1344.73	Joback Method
cpg	1311.85	J/molxK	1389.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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