3«alpha»,17«alpha»,20«alpha»,21-tetrahydroxy-5«

Inchi: InChI=1S/C19H30O5/c20-9-17(23)19(24)6-5-13-14-3-1-10-7-11(21)2-4-12(10)18(14)16(2
InchiKey: XDQNNHYIBSGLRV-HNFTYYAASA-N
Formula: C19H30O5
SMILES: O=C1CC2C(CCC2(O)C(O)CO)C2CCC3CC(O)CCC3C12
Mol. weight [g/mol]: 338.44

Physical Properties

Property code	Value	Unit	Source
gf	-417.04	kJ/mol	Joback Method
hf	-993.11	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	126.59	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	0.873		Crippen Method
mcvol	260.180	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	3059.00		NIST Webbook
rinpol	3059.00		NIST Webbook
tb	1100.09	K	Joback Method
tc	1350.50	K	Joback Method
tf	661.49	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.40	J/mol×K	1100.09	Joback Method
cpg	1111.84	J/mol×K	1141.83	Joback Method
cpg	1134.67	J/mol×K	1183.56	Joback Method
cpg	1158.16	J/mol×K	1225.30	Joback Method
cpg	1182.54	J/mol×K	1267.03	Joback Method
cpg	1208.06	J/mol×K	1308.77	Joback Method
cpg	1234.99	J/mol×K	1350.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248921&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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