

3,20-Bisethylenedioxy-16alpha-hydroxymethyl-5-p

Inchi:	InChI=1S/C26H40O5/c1-23-8-9-26(30-12-13-31-26)15-18(23)4-5-19-20(23)6-7-24(2)21(
InchiKey:	SQUUQRMCBJCKEJ-UHFFFAOYSA-N
Formula:	C26H40O5
SMILES:	CC1(C2C(CO)CC3C4CC=C5CC6(CCC5(C)C4CCC32C)OCCO6)OCCO1
Mol. weight [g/mol]:	432.59
CAS:	103189-18-0

Physical Properties

Property code	Value	Unit	Source
gf	-70.32	kJ/mol	Joback Method
hf	-826.43	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	104.47	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.290		Crippen Method
mcvol	337.090	ml/mol	McGowan Method
pc	1506.98	kPa	Joback Method
tb	1059.95	K	Joback Method
tc	1313.02	K	Joback Method
tf	725.52	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1431.60	J/molxK	1059.95	Joback Method
cpg	1483.71	J/molxK	1102.13	Joback Method
cpg	1541.07	J/molxK	1144.31	Joback Method
cpg	1604.45	J/molxK	1186.49	Joback Method
cpg	1674.62	J/molxK	1228.66	Joback Method
cpg	1752.37	J/molxK	1270.84	Joback Method
cpg	1838.45	J/molxK	1313.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103189180&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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