3«beta»-hydroxy-13-epi-manoyl oxide

Inchi: InChI=1S/C20H34O2/c1-7-18(4)11-8-15-19(5)12-10-16(21)17(2,3)14(19)9-13-20(15,6)22
InchiKey: JJZSRKRSWWPWCJ-RQPVFEQBSA-N
Formula: C20H34O2
SMILES: C=CC1(C)CCC2C(C)(CCC3C(C)(C)C(O)CCC23C)O1
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
hfus	21.34	kJ/mol	Joback Method
logp	4.714		Crippen Method
mcvol	267.520	ml/mol	McGowan Method
rinpol	2239.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2239.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.29	J/mol×K	796.66	Joback Method
cpg	932.72	J/mol×K	834.00	Joback Method
cpg	959.84	J/mol×K	871.33	Joback Method
cpg	988.09	J/mol×K	908.67	Joback Method
cpg	1017.95	J/mol×K	946.01	Joback Method
cpg	1049.87	J/mol×K	983.35	Joback Method
cpg	1084.31	J/mol×K	1020.68	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290432&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices