22(R or S)-17«alpha»(H),21«beta»(H)-Homohopane

Inchi: InChI=1S/C31H54/c1-9-21(2)22-13-18-28(5)23(22)14-19-30(7)25(28)11-12-26-29(6)17-1

InchiKey: QFBGIDMRCNNMIW-UCCGNZTHSA-N

Formula: C31H54

SMILES: CCC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C

Mol. weight [g/mol]: 426.76

Physical Properties

Property code	Value	Unit	Source
hfus	24.46	kJ/mol	Joback Method
logp	9.524		Crippen Method
mcvol	393.350	ml/mol	McGowan Method
rinpol	3088.00		NIST Webbook
rinpol	3088.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1530.77	J/mol×K	945.41	Joback Method
cpg	1580.09	J/mol×K	985.66	Joback Method
cpg	1633.01	J/mol×K	1025.91	Joback Method
cpg	1690.31	J/mol×K	1066.16	Joback Method
cpg	1752.79	J/mol×K	1106.41	Joback Method
cpg	1821.23	J/mol×K	1146.66	Joback Method
cpg	1896.43	J/mol×K	1186.91	Joback Method

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R548622&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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