

22(S or R)-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	3080.00		NIST Webbook
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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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=R548637&Units=SI>
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
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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