17«beta»,21«beta»(H)-hopane

Inchi: InChI=1S/C30H52/c1-20(2)21-12-17-27(5)22(21)13-18-29(7)24(27)10-11-25-28(6)16-9-1
InchiKey: ZRLNBWWGLOPJIC-XDZDYSHNSA-N
Formula: C30H52
SMILES: CC(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]: 412.73

Physical Properties

Property code	Value	Unit	Source
hfus	21.87	kJ/mol	Joback Method
logp	9.134		Crippen Method
mcvol	379.260	ml/mol	McGowan Method
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1454.25	J/mol×K	922.53	Joback Method
cpg	1501.42	J/mol×K	963.21	Joback Method
cpg	1551.88	J/mol×K	1003.89	Joback Method
cpg	1606.44	J/mol×K	1044.56	Joback Method
cpg	1665.90	J/mol×K	1085.24	Joback Method
cpg	1731.08	J/mol×K	1125.92	Joback Method
cpg	1802.80	J/mol×K	1166.60	Joback Method

Sources

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=R261880&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