17«alpha»-22,29,30-trinorhopane

Inchi: InChI=1S/C27H46/c1-23(2)14-8-16-25(4)20(23)13-18-27(6)22(25)11-10-21-24(3)15-7-9-1
InchiKey: WPKYQECPNNWDJY-MSVXTABKSA-N
Formula: C27H46
SMILES: CC1(C)CCCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC3CCC21C
Mol. weight [g/mol]: 370.65

Physical Properties

Property code	Value	Unit	Source
hfus	16.55	kJ/mol	Joback Method
logp	8.252		Crippen Method
mcvol	336.990	ml/mol	McGowan Method
rinpol	2795.00		NIST Webbook
rinpol	2795.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1233.99	J/mol×K	859.00	Joback Method
cpg	1275.45	J/mol×K	900.92	Joback Method
cpg	1319.40	J/mol×K	942.85	Joback Method
cpg	1366.73	J/mol×K	984.77	Joback Method
cpg	1418.31	J/mol×K	1026.69	Joback Method
cpg	1475.05	J/mol×K	1068.61	Joback Method
cpg	1537.82	J/mol×K	1110.54	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R261840&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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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