

17«beta»-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-
InchiKey:	WPKYQECPNNDJY-GSWSGEHQSA-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	2828.00		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

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R261895&Units=SI>

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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