

Verticilla-4(20),7,11-triene

Inchi:	InChI=1S/C20H32/c1-15-7-6-8-16(2)10-14-19-17(3)11-13-18(12-9-15)20(19,4)5/h8,18H,1
InchiKey:	SNPPNYAGNBWZCL-WHMKARLCSA-N
Formula:	C20H32
SMILES:	C=C1CCC=C(C)CCC2=C(C)CCC(CC1)C2(C)C
Mol. weight [g/mol]:	272.47

Physical Properties

Property code	Value	Unit	Source
hfus	18.75	kJ/mol	Joback Method
logp	6.596		Crippen Method
mcvol	258.040	ml/mol	McGowan Method
rinpol	1982.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.97	J/mol×K	721.57	Joback Method
cpg	798.29	J/mol×K	761.06	Joback Method
cpg	823.12	J/mol×K	800.55	Joback Method
cpg	846.58	J/mol×K	840.04	Joback Method
cpg	868.80	J/mol×K	879.54	Joback Method
cpg	889.92	J/mol×K	919.03	Joback Method
cpg	910.07	J/mol×K	958.52	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R626103&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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