

«beta»-Germacrenol

Inchi:	InChI=1S/C15H26O/c1-12(2)14-8-7-13(3)6-5-10-15(4,16)11-9-14/h6,9,11-12,14,16H,5,7H
InchiKey:	RHCTXHCNRLCYBN-ZCSQCZKOSA-N
Formula:	C15H26O
SMILES:	CC1=CCCC(C)(O)C=CC(C(C)C)CC1
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
hfus	15.43	kJ/mol	Joback Method
logp	4.086		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
rinpol	1573.00		NIST Webbook
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rinpol	1573.00		NIST Webbook
ripol	2019.00		NIST Webbook
ripol	2019.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.33	J/mol×K	669.84	Joback Method
cpg	615.86	J/mol×K	705.28	Joback Method
cpg	635.31	J/mol×K	740.71	Joback Method
cpg	653.77	J/mol×K	776.15	Joback Method
cpg	671.33	J/mol×K	811.58	Joback Method
cpg	688.06	J/mol×K	847.02	Joback Method
cpg	704.06	J/mol×K	882.46	Joback Method

Sources

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=R417162&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/ci990307I>

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
ripol:	Polar retention indices

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