

1,6-Germacradien-5«beta»-ol

Other names:	4«beta»-Hydroxy-germacra-1(10),5-diene Germacra-1(10),5-dien-4-«beta»-ol 1,6-Germacradien-5 «beta»-ol (=Germacrene D-4 «beta»-ol) 4b-Hydroxygermacra-1(10),5-diene 1,6-Germacradien-5 «beta»-ol (= germacreneD-4 «beta»-ol), (=1(10),5-germacradien-4 «beta»-ol)
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-GWVGWQBCSA-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	1585.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1586.00		NIST Webbook
ripol	2047.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2064.00		NIST Webbook
ripol	2039.00		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

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R194884&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):

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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