

(2E,4S,7E)-4-Isopropyl-1,7-dimethylcyclodeca-2,7-

Other names:	Germacrene D-4-ol 2,7-Cyclodecadien-1-ol, 1,7-dimethyl-4-(1-methylethyl)-, (2E,4S,7E)- Germacren D-4-ol Germacrene-«delta»-4-ol D-Germacren-4-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,5,7-
InchiKey:	RHCTXHCNRLCYBN-BMCYRRRCSA-N
Formula:	C15H26O
SMILES:	CC1=CCCC(C)(O)C=CC(C(C)C)CC1
Mol. weight [g/mol]:	222.37
CAS:	198991-79-6

Physical Properties

Property code	Value	Unit	Source
gf	-50.70	kJ/mol	Joback Method
hf	-381.77	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.086		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1574.00		NIST Webbook
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rinpol	1557.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1568.00		NIST Webbook
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ripol	2069.00	NIST Webbook
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ripol	2018.00	NIST Webbook
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ripol	2044.00	NIST Webbook
ripol	2049.00	NIST Webbook

ripol	2054.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2057.00		NIST Webbook
ripol	2035.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2018.00		NIST Webbook
tb	669.84	K	Joback Method
tc	882.46	K	Joback Method
tf	331.63	K	Joback Method
vc	0.758	m ³ /kmol	Joback Method

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C198991796&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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