

Germacren-4-ol

Other names:

Germacrene-4-ol
1(10),5-Germacradien-4«beta»-ol

Germacra-1(10),5-dien-4 «alpha»-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-ZCSQCZKOSA-N

Formula: C15H26O

SMILES: CC1=CCCC(C)(O)C=CC(C(C)C)CC1

Mol. weight [g/mol]: 222.37

CAS: 74841-87-5

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
ripol	1576.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1542.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1577.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2050.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74841875&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Non-polar retention indices
ripol:	Polar retention indices

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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