

Ylanga-2,4-(15)-diene

Inchi:	InChI=1S/C15H22/c1-9(2)11-7-8-15(4)12-6-5-10(3)14(15)13(11)12/h5-6,9,11-14H,3,7-8H
InchiKey:	ADVJSMBYHNLGK-CQYKSGMSSA-N
Formula:	C15H22
SMILES:	C=C1C=CC2C3C(C(C)C)CCC2(C)C13
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	305.26	kJ/mol	Joback Method
hf	-29.39	kJ/mol	Joback Method
hfus	19.29	kJ/mol	Joback Method
hvap	47.19	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	4.047		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
tb	555.87	K	Joback Method
tc	770.49	K	Joback Method
tf	323.97	K	Joback Method
vc	0.699	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.38	J/mol×K	555.87	Joback Method
cpg	504.05	J/mol×K	591.64	Joback Method
cpg	524.27	J/mol×K	627.41	Joback Method
cpg	543.20	J/mol×K	663.18	Joback Method
cpg	561.04	J/mol×K	698.95	Joback Method
cpg	577.96	J/mol×K	734.72	Joback Method
cpg	594.13	J/mol×K	770.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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