

Ylangenol

Inchi:	InChI=1S/C15H24O/c1-9(2)11-6-7-15(3)12-5-4-10(8-16)14(15)13(11)12/h4,9,11-14,16H,
InchiKey:	JIXPRNKLOIEGFI-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC(C)C1CCC2(C)C3CC=C(CO)C2C13
Mol. weight [g/mol]:	220.35
CAS:	41610-69-9

Physical Properties

Property code	Value	Unit	Source
gf	105.73	kJ/mol	Joback Method
hf	-277.33	kJ/mol	Joback Method
hfus	24.15	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.243		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1666.40		NIST Webbook
tb	653.87	K	Joback Method
tc	853.56	K	Joback Method
tf	383.63	K	Joback Method
vc	0.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.92	J/molxK	653.87	Joback Method
cpg	594.00	J/molxK	687.15	Joback Method
cpg	611.17	J/molxK	720.43	Joback Method
cpg	627.59	J/molxK	753.72	Joback Method
cpg	643.38	J/molxK	787.00	Joback Method
cpg	658.71	J/molxK	820.28	Joback Method
cpg	673.73	J/molxK	853.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41610699&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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