

«delta»-Ylangene

Inchi:	InChI=1S/C14H22/c1-8(2)10-6-7-11-12-5-4-9(3)13(11)14(10)12/h4-5,8-14H,6-7H2,1-3H3
InchiKey:	UJVZREQMNFOMLV-RVARXAPGSA-N
Formula:	C14H22
SMILES:	CC(C)C1CCC2C3C=CC(C)C2C31
Mol. weight [g/mol]:	190.32

Physical Properties

Property code	Value	Unit	Source
gf	241.54	kJ/mol	Joback Method
hf	-128.57	kJ/mol	Joback Method
hfus	25.23	kJ/mol	Joback Method
hvap	45.65	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.737		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
ripol	1493.00		NIST Webbook
tb	528.92	K	Joback Method
tc	736.57	K	Joback Method
tf	270.88	K	Joback Method
vc	0.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.16	J/mol×K	528.92	Joback Method
cpg	474.31	J/mol×K	563.53	Joback Method
cpg	496.03	J/mol×K	598.14	Joback Method
cpg	516.41	J/mol×K	632.75	Joback Method
cpg	535.53	J/mol×K	667.35	Joback Method
cpg	553.47	J/mol×K	701.96	Joback Method
cpg	570.32	J/mol×K	736.57	Joback Method
dvisc	0.0006844	Paxs	270.88	Joback Method
dvisc	0.0008842	Paxs	313.89	Joback Method

dvisc	0.0010740	Paxs	356.89	Joback Method
dvisc	0.0012511	Paxs	399.90	Joback Method
dvisc	0.0014148	Paxs	442.91	Joback Method
dvisc	0.0015655	Paxs	485.91	Joback Method
dvisc	0.0017039	Paxs	528.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514104&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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