5-epi-Paradisol

Inchi: InChI=1S/C15H26O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h12-13,16H,1,5-10H
InchiKey: DPQYOKVMVCQHMY-APIJFGDWSA-N
Formula: C15H26O
SMILES: C=C(C)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	64.59	kJ/mol	Joback Method
hf	-278.76	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
ripol	2154.00		NIST Webbook
ripol	2154.00		NIST Webbook
tb	653.04	K	Joback Method
tc	865.92	K	Joback Method
tf	365.03	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.33	J/mol×K	653.04	Joback Method
cpg	613.82	J/mol×K	688.52	Joback Method
cpg	633.38	J/mol×K	724.00	Joback Method
cpg	652.21	J/mol×K	759.48	Joback Method
cpg	670.53	J/mol×K	794.96	Joback Method
cpg	688.57	J/mol×K	830.44	Joback Method

cpg	706.54	J/mol×K	865.92	Joback Method

Sources

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=R585245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume