

cis-Pinocarveol

Inchi:

InChI=1S/C10H16O/c1-6-8-4-7(5-9(6)11)10(8,2)3/h7-9,11H,1,4-5H2,2-3H3/t7-,8+,9-/m1/

InchiKey:

LCYXQUJDODZYIJ-HRDYMLBCSA-N

Formula:

C10H16O

SMILES:

C=C1C(O)CC2CC1C2(C)C

Mol. weight [g/mol]:

152.23

Physical Properties

Property code	Value	Unit	Source
gf	38.07	kJ/mol	Joback Method
hf	-203.72	kJ/mol	Joback Method
hfus	14.60	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	1184.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1175.00		NIST Webbook
tb	528.19	K	Joback Method
tc	723.06	K	Joback Method
tf	324.74	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.96	J/mol×K	528.19	Joback Method
cpg	350.83	J/mol×K	560.67	Joback Method
cpg	364.79	J/mol×K	593.15	Joback Method
cpg	377.93	J/mol×K	625.63	Joback Method
cpg	390.35	J/mol×K	658.11	Joback Method
cpg	402.17	J/mol×K	690.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R603531&Units=SI
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

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

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