

Isopinocarveol

Other names:	cis-Pinocarveol Bicyclo[3.1.1]heptan-3-ol, 6,6-dimethyl-2-methylene-, (1«alpha»,3«beta»,5«alpha»)- 2(10)-Pinen-3-ol, cis- (Z)-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
InchiKey:	LCYXQUJDODZYIJ-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	<chem>C=C1C(O)CC2CC1C2(C)C</chem>
Mol. weight [g/mol]:	152.23
CAS:	6712-79-4

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
h vap	52.92	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
m cvol	131.610	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1139.00		NIST Webbook

rinpol	1160.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1139.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1640.00		NIST Webbook
tb	528.19	K	Joback Method
tc	723.06	K	Joback Method
tf	324.74	K	Joback Method
vc	0.500	m ³ /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
cpg	413.48	J/mol×K	723.06	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=C6712794&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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