

Bicyclo[3.1.1]heptan-3-ol, 6,6-dimethyl-2-methylene-

Other names:	Pinocarveol 2(10)-Pinen-3-ol 6,6-dimethyl-2-methylenebicyclo[3.1.1]heptan-3-ol
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:	C=C1C(O)CC2CC1C2(C)C
Mol. weight [g/mol]:	152.23
CAS:	5947-36-4

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
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	1128.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1139.00		NIST Webbook

ripol	1147.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1146.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1637.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1654.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1653.00		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:

<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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5947364&Units=SI>

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

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