

trans-2-Pinanol

Other names:	Bicyclo(3.1.1)heptan-2-ol, 2,6,6-trimethyl-, (1«alpha»,2«beta»,5«alpha»)-Pinan-2«beta»-ol 2-Pinanol, trans- 2,6,6-Trimethylbicyclo(3.1.1)heptan-2-ol, (1«alpha»,2«beta»,5«alpha»)- 2,6,6-Trimethylbicyclo[3.1.1]heptan-2-ol-, (1R,2R,5S)-rel-(E)-Pinan-2-ol trans-Pinan-2-ol trans-Pinene hydrate (E)-Pinene hydrate NSC 2326
Inchi:	InChI=1S/C10H18O/c1-9(2)7-4-5-10(3,11)8(9)6-7/h7-8,11H,4-6H2,1-3H3/t7?,8?,10-/m1/s
InchiKey:	YYWZKGZIIKPPJZ-SFVIPPHHSA-N
Formula:	C10H18O
SMILES:	CC1(O)CCC2CC1C2(C)C
Mol. weight [g/mol]:	154.25
CAS:	4948-29-2

Physical Properties

Property code	Value	Unit	Source
gf	-20.50	kJ/mol	Joback Method
hf	-272.72	kJ/mol	Joback Method
hfus	9.46	kJ/mol	Joback Method
hvap	51.61	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.194		Crippen Method
mccvol	135.910	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1088.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1140.00		NIST Webbook

rinpol	1138.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1126.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1522.00		NIST Webbook
tb	529.27	K	Joback Method
tc	730.21	K	Joback Method
tf	334.96	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.30	J/mol×K	529.27	Joback Method
cpg	370.25	J/mol×K	562.76	Joback Method
cpg	385.05	J/mol×K	596.25	Joback Method
cpg	398.92	J/mol×K	629.74	Joback Method
cpg	412.02	J/mol×K	663.23	Joback Method
cpg	424.55	J/mol×K	696.72	Joback Method
cpg	436.70	J/mol×K	730.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4948292&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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