Trans-2-pinanol

Other names: (E)-Pinan-2-ol
(E)-Pinene hydrate
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-
2-Pinanol, trans-
Bicyclo(3.1.1)heptan-2-ol, 2,6,6-trimethyl-, (1«alpha»,2«beta»,5«alpha»)-
NSC 2326
Pinan-2«beta»-ol
trans-Pinan-2-ol
trans-Pinene hydrate

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-/m0/s

InchiKey: YYWZKGZIIKPPJZ-SFVIPPHHSA-N

Formula: C10H18O

SMILES: CC1(C)C2CC[C@](C)(O)C1C2

Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
hfus	9.46	kJ/mol	Joback Method
logp	2.194		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
rinpol	1140.00		NIST Webbook
rinpol	1118.00		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	1088.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1137.00		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	1110.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1120.00	NIST Webbook
ripol	1522.00	NIST Webbook
ripol	1522.00	NIST Webbook

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
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices