(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene

Other names:	1R-«alpha»-Pinene Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, (1R)- 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene-, (1R,5R)- d-«alpha»-Pinene 1R-(+)-«alpha»-Pinene (R)-«alpha»-Pinene «alpha»-Pinene, (D)- Dextro-alpha-pinene (+)-pin-2(3)-ene «alpha»-Pinene(dextro)
Inchi:	InChI=1S/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h4,8-9H,5-6H2,1-3H3/t8-,9?/m1/s1
InchiKey:	GRWFGVWFFZKLTI-VEDVMXKPSA-N
Formula:	C10H16
SMILES:	CC1=CCC2CC1C2(C)C
Mol. weight [g/mol]:	136.23
CAS:	7785-70-8

Physical Properties

Property code	Value	Unit	Source
chl	-6156.80	kJ/mol	NIST Webbook
gf	149.85	kJ/mol	Joback Method
hf	-69.08	kJ/mol	Joback Method
hfus	11.43	kJ/mol	Joback Method
hvap	37.35	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	937.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	935.00		NIST Webbook
ripol	1010.00		NIST Webbook
ripol	1016.00		NIST Webbook

tb	428.20	K	NIST Webbook
tc	654.83	K	Joback Method
tf	267.76	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.36	J/mol×K	445.66	Joback Method
cpg	292.47	J/mol×K	480.52	Joback Method
cpg	309.23	J/mol×K	515.38	Joback Method
cpg	324.78	J/mol×K	550.25	Joback Method
cpg	339.25	J/mol×K	585.11	Joback Method
cpg	352.77	J/mol×K	619.97	Joback Method
cpg	365.49	J/mol×K	654.83	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7785708&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chl: Standard liquid enthalpy of combustion
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