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

Other names: 1S-«alpha»-Pinene
(-)-«alpha»-Pinene
L-«alpha»-Pinene
Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, (1S)-
2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene-, (1S,5S)-
«alpha»-Pinene, (-)-
(1S)-(-)-«alpha»-Pinene
1S-(-)-a-pinene
(-)-pin-2(3)-ene

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: 7785-26-4

Physical Properties

Property code	Value	Unit	Source
chl	-6150.50	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	956.02		NIST Webbook
rinpol	941.76		NIST Webbook
rinpol	945.19		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	952.30		NIST Webbook
rinpol	955.94		NIST Webbook
rinpol	959.63		NIST Webbook
rinpol	963.45		NIST Webbook
rinpol	967.39		NIST Webbook
rinpol	928.69		NIST Webbook

rinpol	931.87		NIST Webbook
rinpol	935.08		NIST Webbook
rinpol	938.37		NIST Webbook
rinpol	941.85		NIST Webbook
rinpol	945.26		NIST Webbook
rinpol	948.88		NIST Webbook
rinpol	952.43		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	922.57		NIST Webbook
rinpol	925.64		NIST Webbook
rinpol	928.73		NIST Webbook
rinpol	931.91		NIST Webbook
rinpol	935.13		NIST Webbook
rinpol	938.44		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	948.69		NIST Webbook
ripol	1030.00		NIST Webbook
ripol	1030.00		NIST Webbook
ripol	1029.00		NIST Webbook
ripol	1029.00		NIST Webbook
ripol	1030.00		NIST Webbook
ripol	1008.00		NIST Webbook
tb	428.20	K	NIST Webbook
tc	654.83	K	Joback Method
tf	218.39 ± 0.15	K	NIST Webbook
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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7785264&Units=SI

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