Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-

Other names: 2(10)-Pinene, (1S,5S)-(-)-
(-)-«beta»-Pinene
(-)-2(10)-Pinene
L-«beta»-Pinene
(1S)-(-)-«beta»-Pinene
laevo-«beta»-Pinene
6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane-, (S)-
(-)-beta-Pinene
Bicyclo(3.1.1)heptane, 6,6-dimethyl-2-methylene-, (1S,5S)-
(-)-Pin-2(10)-ene
«beta»-Pinene-(1S)-(-)

Inchi: InChI=1S/C10H16/c1-7-4-5-8-6-9(7)10(8,2)3/h8-9H,1,4-6H2,2-3H3

InchiKey: WTARULDDTDQWMU-UHFFFAOYSA-N

Formula: C10H16

SMILES: C=C1CCC2CC1C2(C)C

Mol. weight [g/mol]: 136.23

CAS: 18172-67-3

Physical Properties

Property code	Value	Unit	Source
gf	182.60	kJ/mol	Joback Method
hf	-31.15	kJ/mol	Joback Method
hfus	9.44	kJ/mol	Joback Method
hvap	36.55	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
tb	439.20	K	NIST Webbook
tc	648.22	K	Joback Method
tf	268.16	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.71	J/mol×K	440.68	Joback Method
cpg	291.03	J/mol×K	475.27	Joback Method
cpg	308.01	J/mol×K	509.86	Joback Method
cpg	323.77	J/mol×K	544.45	Joback Method
cpg	338.45	J/mol×K	579.04	Joback Method
cpg	352.17	J/mol×K	613.63	Joback Method
cpg	365.06	J/mol×K	648.22	Joback Method
hvapt	46.10	kJ/mol	366.00	NIST Webbook
hvapt	44.90	kJ/mol	328.00	NIST Webbook

Sources

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=C18172673&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume