Bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde, 6,6-dimethyl-

Other names:	2-Norpinene-2-carboxaldehyde, 6,6-dimethyl-
	Myrtenal
	Benihinal
	6,6-Dimethylbicyclo(3.1.1)hept-2-ene-2-carboxaldehyde
	2-Formyl-6,6-dimethylbicyclo(3.1.1)hept-2-ene
	6,6-Dimethyl-bicyclo[3,1,1]hept-2-ene-2-carboxaldehyde
	6,6-dimethyl-bicyclo[3.1.1]hept-2-ene-2-carboxaldehyde (myrtenal)
	pin-2-ene-1-carbaldehyde
Inchi:	InChI=1S/C10H14O/c1-10(2)8-4-3-7(6-11)9(10)5-8/h3,6,8-9H,4-5H2,1-2H3
InchiKey:	KMRMUZKLFIEVAO-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC1(C)C2CC=C(C=O)C1C2
Mol. weight [g/mol]:	150.22
CAS:	564-94-3

Physical Properties

Property code	Value	Unit	Source
gf	50.33	kJ/mol	Joback Method
hf	-154.66	kJ/mol	Joback Method
hfus	13.72	kJ/mol	Joback Method
hvap	44.07	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
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tb	493.70	K	NIST Webbook
tc	708.63	K	Joback Method
tf	309.76	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.50	J/mol×K	494.32	Joback Method
cpg	315.43	J/mol×K	530.04	Joback Method
cpg	330.16	J/mol×K	565.76	Joback Method
cpg	343.83	J/mol×K	601.47	Joback Method
cpg	356.59	J/mol×K	637.19	Joback Method
cpg	368.56	J/mol×K	672.91	Joback Method
cpg	379.90	J/mol×K	708.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C564943&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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