Bicyclo[3.1.1]heptane-2-carboxaldehyde, 6,6-dimethyl-

Other names: Myrtanal
10-Pinanal
2-Norpinanecarboxaldehyde, 6,6-dimethyl-
Myrtenal, dihydro-
6,6-dimethylbicyclo[3.1.1]heptane-2-carbaldehyde

Inchi: InChI=1S/C10H16O/c1-10(2)8-4-3-7(6-11)9(10)5-8/h6-9H,3-5H2,1-2H3

InchiKey: OOCLVMCVOWKECB-UHFFFAOYSA-N

Formula: C10H16O

SMILES: CC1(C)C2CCC(C=O)C1C2

Mol. weight [g/mol]: 152.23

CAS: 4764-14-1

Physical Properties

Property code	Value	Unit	Source
gf	22.29	kJ/mol	Joback Method
hf	-221.31	kJ/mol	Joback Method
hfus	13.96	kJ/mol	Joback Method
hvap	42.80	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1197.60		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1188.00		NIST Webbook
ripol	1543.00		NIST Webbook
tb	485.51	K	Joback Method
tc	696.20	K	Joback Method
tf	292.24	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.83	J/mol×K	485.51	Joback Method
cpg	333.89	J/mol×K	520.63	Joback Method
cpg	350.66	J/mol×K	555.74	Joback Method
cpg	366.27	J/mol×K	590.86	Joback Method
cpg	380.86	J/mol×K	625.97	Joback Method
cpg	394.56	J/mol×K	661.09	Joback Method
cpg	407.51	J/mol×K	696.20	Joback Method

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=C4764141&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
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