1-Cyclohexene-1-carboxaldehyde, 4-(1-methylethyl)-

Other names: Phellandral
4-Isopropyl-1-cyclohexene-1-carbaldehyde
4-[1-Methylethyl]-1-cyclohexene-1-carboxaldehyde
p-Menth-1-en-7-al
4-isopropylcyclohexenecarbaldehyde

Inchi: InChI=1S/C10H16O/c1-8(2)10-5-3-9(7-11)4-6-10/h3,7-8,10H,4-6H2,1-2H3

InchiKey: AEVLWICMAHGAMS-UHFFFAOYSA-N

Formula: C10H16O

SMILES: CC(C)C1CC=C(C=O)CC1

Mol. weight [g/mol]: 152.23

CAS: 21391-98-0

Physical Properties

Property code	Value	Unit	Source
gf	-23.86	kJ/mol	Joback Method
hf	-239.96	kJ/mol	Joback Method
hfus	13.09	kJ/mol	Joback Method
hvap	45.57	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1281.00		NIST Webbook

rinpol	1281.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1271.20		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1252.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1715.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1759.00		NIST Webbook
tb	500.11	K	Joback Method
tc	710.00	K	Joback Method
tf	250.12	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.82	J/mol×K	500.11	Joback Method
cpg	388.15	J/mol×K	675.02	Joback Method
cpg	374.78	J/mol×K	640.04	Joback Method
cpg	360.59	J/mol×K	605.06	Joback Method
cpg	345.55	J/mol×K	570.07	Joback Method
cpg	329.63	J/mol×K	535.09	Joback Method
cpg	400.72	J/mol×K	710.00	Joback Method
dvisc	0.0002874	Pa×s	500.11	Joback Method
dvisc	0.0003747	Pa×s	458.44	Joback Method
dvisc	0.0005151	Pa×s	416.78	Joback Method
dvisc	0.0007601	Pa×s	375.12	Joback Method
dvisc	0.0012360	Pa×s	333.45	Joback Method
dvisc	0.0023094	Pa×s	291.78	Joback Method
dvisc	0.0053140	Pa×s	250.12	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=C21391980&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
dvisc: Dynamic viscosity
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