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

Other names: 1-Cyclohexene-1-carboxaldehyde, 4-isopropenyl-
Perilla aldehyde
Perillal
Perillaldehyde
p-Mentha-1,8-dien-7-al
Dihydrocuminyl aldehyde
4-Isopropenyl-1-cyclohexene-1-carboxaldehyde
para-Mentha-1,8-dien-7-al
Perillyl aldehyde
NSC 138642
p-Isopropenyl cyclohexencarbaldehyde
perrilaldehyde
Perrilla aldehyde
4-isopropenylcyclohex-1-enecarbaldehyde

Inchi: InChI=1S/C10H14O/c1-8(2)10-5-3-9(7-11)4-6-10/h3,7,10H,1,4-6H2,2H3

InchiKey: RUMOYJJNUMEFDD-UHFFFAOYSA-N

Formula: C10H14O

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

Mol. weight [g/mol]: 150.22

CAS: 2111-75-3

Physical Properties

Property code	Value	Unit	Source
hfus	14.02	kJ/mol	Joback Method
hvap	61.27	kJ/mol	Cheméo Relay (1.0)
ie	10.10	eV	NIST Webbook
log10ws	-2.51		Cheméo Relay (1.0)
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1294.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1268.00		NIST Webbook

rinpol	1246.00	NIST Webbook
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ripol	1797.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1776.00		NIST Webbook
tb	508.11	K	Cheméo Relay (1.0)
tf	220.90	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-4.10100e+01
Coeff. B	9.14820e-01
Coeff. C	-5.39640e-04
Coeff. D	1.13800e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2111753&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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