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
gf	57.87	kJ/mol	Joback Method
hf	-119.04	kJ/mol	Joback Method
hfus	14.02	kJ/mol	Joback Method
hvap	45.37	kJ/mol	Joback Method
ie	10.10	eV	NIST Webbook
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1253.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1271.00		NIST Webbook

rinpol	1290.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1272.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1252.00	NIST Webbook
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ripol	1814.00	NIST Webbook

ripol	1818.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1785.00		NIST Webbook
tb	497.11	K	Joback Method
tc	710.87	K	Joback Method
tf	249.40	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.38	J/mol×K	497.11	Joback Method
cpg	310.40	J/mol×K	532.74	Joback Method
cpg	325.51	J/mol×K	568.36	Joback Method
cpg	339.74	J/mol×K	603.99	Joback Method
cpg	353.13	J/mol×K	639.62	Joback Method
cpg	365.70	J/mol×K	675.25	Joback Method
cpg	377.49	J/mol×K	710.87	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C2111753&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy

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