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	1274.00		NIST Webbook
rinpol	1279.20		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1272.00		NIST Webbook

rinpol	1254.00	NIST Webbook
rinpol	1257.00	NIST Webbook
rinpol	1268.00	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1248.00	NIST Webbook
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ripol	1807.00	NIST Webbook

ripol	1807.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1781.00		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

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
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
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

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