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

Other names:	L-Perillaldehyde
	1-Cyclohexene-1-carboxaldehyde, 4-isopropenyl-, (S)-(-)-
	(-)-Perillaldehyde
	(4S)-p-Mentha-1,8-dien-7-al
	(S)-(-)-Perillaldehyde
	4-Isopropenyl-1-cyclohexene-1-carbaldehyde, (S)-
	(S)-(-)-Perillic aldehyde
	1-Cyclohexene-1-carboxaldehyde, 4-(1-methylethenyl)-, (4S)-
	(-)-Perilla aldehyde
	1-perillaldehyde
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:	18031-40-8

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
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1243.00		NIST Webbook
rinpol	1243.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1774.00		NIST Webbook
ripol	1768.00		NIST Webbook
ripol	1776.00		NIST Webbook
ripol	1777.00		NIST Webbook
ripol	1776.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.70	K	1.30	NIST Webbook

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=C18031408&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume