2-ISOPROPYL-5-METHYLHEX-2-ENAL

Other names: 2-Isopropyl-5-methyl-2-hexenal
2-Hexenal, 5-methyl-2-(1-methylethyl)-
2-Hexen-1-al, 2-isopropyl-5-methyl-
2-Hexen-1-al, 5-methyl-2-(1-methylethyl)-
Isodihydrolavandulyl aldehyde
2-Isopropyl-5-methyl-2-hexen-1-al
Inchi: InChI=1S/C10H18O/c1-8(2)5-6-10(7-11)9(3)4/h6-9H,5H2,1-4H3/b10-6+
InchiKey: IOLQAHFPDADCHJ-POHAHGRESA-N
Formula: C10H18O
SMILES: CC(C)C/C=C(/C=O)C(C)C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
hfus	15.79	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Cheméo Relay (1.0)
ie	9.35	eV	Cheméo Relay (1.0)
logp	2.814		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
rinpol	1100.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1373.00		NIST Webbook
tb	457.23	K	Cheméo Relay (1.0)
tf	228.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.28	J/mol×K	480.02	Joback Method
cpg	341.03	J/mol×K	511.21	Joback Method
cpg	355.07	J/mol×K	542.39	Joback Method
cpg	368.41	J/mol×K	573.58	Joback Method
cpg	381.09	J/mol×K	604.76	Joback Method
cpg	393.14	J/mol×K	635.95	Joback Method
cpg	404.58	J/mol×K	667.13	Joback Method

Sources

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=C35158259&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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