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)CC=C(C=O)C(C)C

Mol. weight [g/mol]: 154.25

CAS: 35158-25-9

Physical Properties

Property code	Value	Unit	Source
gf	0.59	kJ/mol	Joback Method
hf	-238.44	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	43.84	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.814		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1106.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1100.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1373.00		NIST Webbook
tb	480.02	K	Joback Method
tc	667.13	K	Joback Method
tf	195.42	K	Joback Method

vc	0.582	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35158259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume