2-ISOPROPYL-5-METHYLHEXYL ACETATE

Other names: 2-Isopropyl-5-methylhexyl acetate
Tetrahydrolavandulyl acetate
1-Hexanol, 2-isopropyl-5-methyl-, acetate
Inchi: InChI=1S/C12H24O2/c1-9(2)6-7-12(10(3)4)8-14-11(5)13/h9-10,12H,6-8H2,1-5H3
InchiKey: QLFSGYMLVZGFJT-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CC(=O)OCC(CCC(C)C)C(C)C
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
af	0.5505		Cheméo Relay (1.0)
hf	-622.61	kJ/mol	Cheméo Relay (1.0)
hfus	19.05	kJ/mol	Joback Method
hvap	64.47	kJ/mol	Cheméo Relay (1.0)
ie	9.36	eV	Cheméo Relay (1.0)
log10ws	-3.76		Cheméo Relay (1.0)
logp	3.258		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	1254.30		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
tb	497.13	K	Cheméo Relay (1.0)
tc	664.58	K	Cheméo Relay (1.0)
tf	220.10	K	Cheméo Relay (1.0)
vc	0.663	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.98	J/mol×K	548.93	Joback Method
cpg	481.72	J/mol×K	578.83	Joback Method
cpg	497.75	J/mol×K	608.74	Joback Method

cpg	513.09	J/mol×K	638.64	Joback Method
cpg	527.75	J/mol×K	668.55	Joback Method
cpg	541.73	J/mol×K	698.45	Joback Method
cpg	555.06	J/mol×K	728.36	Joback Method
dvisc	0.0095948	Pa×s	252.16	Joback Method
dvisc	0.0027490	Pa×s	301.62	Joback Method
dvisc	0.0011201	Pa×s	351.08	Joback Method
dvisc	0.0005697	Pa×s	400.54	Joback Method
dvisc	0.0003362	Pa×s	450.01	Joback Method
dvisc	0.0002202	Pa×s	499.47	Joback Method
dvisc	0.0001557	Pa×s	548.93	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40853552&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

Latest version available from:
https://www.chemeo.com/cid/75-296-1/2-ISOPROPYL-5-METHYLHEXYL-ACETATE.pdf
Generated by Cheméo on 2026-07-22 01:21:18.602137207 +0000 UTC m=+194374.444022589.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.