

Lavandulyl acetate

Other names:	(-)-Lavandulyl acetate Lavendulyl acetate 4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, acetate, (R)- (R)-2-isopropenyl-5-methylhex-4-enyl acetate
Inchi:	InChI=1S/C12H20O2/c1-9(2)6-7-12(10(3)4)8-14-11(5)13/h6,12H,3,7-8H2,1-2,4-5H3
InchiKey:	HYNGAVZPWWXQIU-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	C=C(C)C(CC=C(C)C)COC(C)=O
Mol. weight [g/mol]:	196.29
CAS:	20777-39-3

Physical Properties

Property code	Value	Unit	Source
gf	-35.24	kJ/mol	Joback Method
hf	-318.02	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	50.52	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.098		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	1273.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1277.00		NIST Webbook
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rinpol	1273.00		NIST Webbook
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ripol	1584.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1584.00		NIST Webbook
tb	550.41	K	Joback Method
tc	739.62	K	Joback Method
tf	247.40	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.81	J/mol×K	550.41	Joback Method
cpg	441.39	J/mol×K	581.95	Joback Method
cpg	456.21	J/mol×K	613.48	Joback Method
cpg	470.31	J/mol×K	645.02	Joback Method
cpg	483.71	J/mol×K	676.55	Joback Method
cpg	496.44	J/mol×K	708.09	Joback Method
cpg	508.52	J/mol×K	739.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20777393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	http://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

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