

(E)-Sesquilavandulyl acetate

Inchi: InChI=1S/C17H28O2/c1-13(2)8-7-9-15(5)10-11-17(14(3)4)12-19-16(6)18/h8,10,17H,3,7,
InchiKey: WKGRFMQERVPGIC-XNTDXEJSSA-N
Formula: C17H28O2
SMILES: C=C(C)C(CC=C(C)CCC=C(C)C)COC(C)=O
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	78.53	kJ/mol	Joback Method
hf	-313.79	kJ/mol	Joback Method
hfus	34.24	kJ/mol	Joback Method
hvap	61.69	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.825		Crippen Method
mcvol	244.930	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	1809.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
tb	668.85	K	Joback Method
tc	857.99	K	Joback Method
tf	284.71	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.44	J/molxK	668.85	Joback Method
cpg	683.28	J/molxK	700.37	Joback Method
cpg	700.22	J/molxK	731.90	Joback Method
cpg	716.29	J/molxK	763.42	Joback Method

cpg	731.55	J/mol×K	794.94	Joback Method
cpg	746.03	J/mol×K	826.46	Joback Method
cpg	759.78	J/mol×K	857.99	Joback Method

Sources

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=R204401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mvol:	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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