

Lavandulyl 2-methylbutanoate

Inchi:	InChI=1S/C16H28O2/c1-7-13(5)15(10-9-12(3)4)11-18-16(17)14(6)8-2/h9,14-15H,5,7-8,1
InchiKey:	WKOIIBFHNHYDRV-UHFFFAOYSA-N
Formula:	C16H28O2
SMILES:	<chem>C=C(CC)C(CC=C(C)C)COC(=O)C(C)CC</chem>
Mol. weight [g/mol]:	252.39
CAS:	147044-46-0

Physical Properties

Property code	Value	Unit	Source
gf	-4.00	kJ/mol	Joback Method
hf	-405.86	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	59.04	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.514		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1489.00		NIST Webbook
ripol	1761.00		NIST Webbook
tb	641.49	K	Joback Method
tc	826.32	K	Joback Method
tf	277.48	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.59	J/molxK	641.49	Joback Method
cpg	650.59	J/molxK	672.29	Joback Method
cpg	667.71	J/molxK	703.10	Joback Method
cpg	683.98	J/molxK	733.90	Joback Method

cpg	699.42	J/mol×K	764.71	Joback Method
cpg	714.08	J/mol×K	795.51	Joback Method
cpg	727.98	J/mol×K	826.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C147044460&Units=SI

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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