

Lavandulyl isobutyrate

Inchi:	InChI=1S/C14H24O2/c1-10(2)7-8-13(11(3)4)9-16-14(15)12(5)6/h7,12-13H,3,8-9H2,1-2,4H
InchiKey:	HPBLXFPAJRUKY-UHFFFAOYSA-N
Formula:	C14H24O2
SMILES:	C=C(C)C(CC=C(C)C)COC(=O)C(C)C
Mol. weight [g/mol]:	224.34
CAS:	51117-20-5

Physical Properties

Property code	Value	Unit	Source
gf	-20.84	kJ/mol	Joback Method
hf	-364.58	kJ/mol	Joback Method
hfus	24.06	kJ/mol	Joback Method
hvap	54.59	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.734		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	1404.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1417.30		NIST Webbook
ripol	1677.00		NIST Webbook
tb	595.73	K	Joback Method
tc	784.18	K	Joback Method
tf	254.94	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.35	J/mol×K	595.73	Joback Method
cpg	543.47	J/mol×K	627.14	Joback Method
cpg	559.75	J/mol×K	658.55	Joback Method
cpg	575.21	J/mol×K	689.96	Joback Method
cpg	589.90	J/mol×K	721.36	Joback Method

cpg	603.83	J/mol×K	752.77	Joback Method
cpg	617.03	J/mol×K	784.18	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=C51117205&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
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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