Lavandulyl butyrate

Inchi: InChI=1S/C14H24O2/c1-6-7-14(15)16-10-13(12(4)5)9-8-11(2)3/h8,13H,4,6-7,9-10H2,1-3
InchiKey: ROJSUZRYGHOLJL-UHFFFAOYSA-N
Formula: C14H24O2
SMILES: C=C(C)C(CC=C(C)C)COC(=O)CCC
Mol. weight [g/mol]: 224.34
CAS: 59550-35-5

Physical Properties

Property code	Value	Unit	Source
gf	-18.40	kJ/mol	Joback Method
hf	-359.30	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	54.97	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.878		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	1459.70		NIST Webbook
rinpol	1459.70		NIST Webbook
tb	596.17	K	Joback Method
tc	781.23	K	Joback Method
tf	269.94	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.99	J/mol×K	596.17	Joback Method
cpg	542.76	J/mol×K	627.01	Joback Method
cpg	558.71	J/mol×K	657.86	Joback Method
cpg	573.90	J/mol×K	688.70	Joback Method
cpg	588.33	J/mol×K	719.54	Joback Method
cpg	602.04	J/mol×K	750.38	Joback Method
cpg	615.07	J/mol×K	781.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59550355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume