Lavandulyl propionate

Inchi: InChI=1S/C13H22O2/c1-6-13(14)15-9-12(11(4)5)8-7-10(2)3/h7,12H,4,6,8-9H2,1-3,5H3
InchiKey: NQCUUXYGJVLXAT-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: C=C(C)C(CC=C(C)C)COC(=O)CC
Mol. weight [g/mol]: 210.31
CAS: 59550-34-4

Physical Properties

Property code	Value	Unit	Source
gf	-26.82	kJ/mol	Joback Method
hf	-338.66	kJ/mol	Joback Method
hfus	24.99	kJ/mol	Joback Method
hvap	52.75	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.488		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	1375.00		NIST Webbook
rinpol	1375.00		NIST Webbook
tb	573.29	K	Joback Method
tc	760.33	K	Joback Method
tf	258.67	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.11	J/mol×K	573.29	Joback Method
cpg	491.31	J/mol×K	604.46	Joback Method
cpg	506.74	J/mol×K	635.64	Joback Method
cpg	521.42	J/mol×K	666.81	Joback Method
cpg	535.37	J/mol×K	697.98	Joback Method
cpg	548.63	J/mol×K	729.15	Joback Method
cpg	561.21	J/mol×K	760.33	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=C59550344&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume