Lavandulyl isobutanoate

Inchi: InChI=1S/C14H26O2/c1-10(2)7-8-13(11(3)4)9-16-14(15)12(5)6/h8,10-12H,7,9H2,1-6H3/
InchiKey: ZEOZKJMELMMXOU-JYRVWZFOSA-N
Formula: C14H26O2
SMILES: CC(C)CC=C(COC(=O)C(C)C)C(C)C
Mol. weight [g/mol]: 226.35

Physical Properties

Property code	Value	Unit	Source
gf	-102.57	kJ/mol	Joback Method
hf	-485.50	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	54.79	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.814		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1435.00		NIST Webbook
tb	598.73	K	Joback Method
tc	784.49	K	Joback Method
tf	255.66	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.26	J/mol×K	598.73	Joback Method
cpg	566.01	J/mol×K	629.69	Joback Method
cpg	582.92	J/mol×K	660.65	Joback Method
cpg	599.01	J/mol×K	691.61	Joback Method
cpg	614.30	J/mol×K	722.57	Joback Method
cpg	628.82	J/mol×K	753.53	Joback Method

cpg	642.60	J/mol×K	784.49	Joback Method

Sources

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=R577487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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