Lavandulyl caproate

Inchi: InChI=1S/C16H28O2/c1-6-7-8-9-16(17)18-12-15(14(4)5)11-10-13(2)3/h10,15H,4,6-9,11-
InchiKey: XIHQQRPPPPVGNN-UHFFFAOYSA-N
Formula: C16H28O2
SMILES: C=C(C)C(CC=C(C)C)COC(=O)CCCCC
Mol. weight [g/mol]: 252.39
CAS: 59550-36-6

Physical Properties

Property code	Value	Unit	Source
gf	-1.56	kJ/mol	Joback Method
hf	-400.58	kJ/mol	Joback Method
hfus	32.76	kJ/mol	Joback Method
hvap	59.43	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.659		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	1649.50		NIST Webbook
rinpol	1649.50		NIST Webbook
tb	641.93	K	Joback Method
tc	823.82	K	Joback Method
tf	292.48	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.18	J/mol×K	641.93	Joback Method
cpg	649.86	J/mol×K	672.25	Joback Method
cpg	666.69	J/mol×K	702.56	Joback Method
cpg	682.71	J/mol×K	732.88	Joback Method
cpg	697.93	J/mol×K	763.19	Joback Method
cpg	712.40	J/mol×K	793.51	Joback Method
cpg	726.14	J/mol×K	823.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59550366&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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