Lavandulyle 2-methylbutyrate

Other names: Lavandulyl 2-methylbutyrate
Inchi: InChI=1S/C15H26O2/c1-7-13(6)15(16)17-10-14(12(4)5)9-8-11(2)3/h13-14H,2,4,7-10H2,1
InchiKey: IBKFLDWCDDVSDC-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: C=C(C)CCC(COC(=O)C(C)CC)C(=C)C
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-4.80	kJ/mol	Joback Method
hf	-377.01	kJ/mol	Joback Method
hfus	25.17	kJ/mol	Joback Method
hvap	56.18	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.124		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1490.00		NIST Webbook
ripol	1759.00		NIST Webbook
tb	611.13	K	Joback Method
tc	793.92	K	Joback Method
tf	269.53	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.03	J/mol×K	611.13	Joback Method
cpg	594.52	J/mol×K	641.60	Joback Method
cpg	611.17	J/mol×K	672.06	Joback Method
cpg	627.02	J/mol×K	702.53	Joback Method

cpg	642.09	J/mol×K	732.99	Joback Method
cpg	656.39	J/mol×K	763.46	Joback Method
cpg	669.96	J/mol×K	793.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232783&Units=SI

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