TRIFLUOROACETYL-LAVANDULOL

Other names: (.+/-.)-Lavandulol, trifluoroacetate
Inchi: InChI=1S/C12H17F3O2/c1-8(2)5-6-10(9(3)4)7-17-11(16)12(13,14)15/h5,10H,3,6-7H2,1-2
InchiKey: NMBAKMPLONJXSQ-UHFFFAOYSA-N
Formula: C12H17F3O2
SMILES: C=C(C)C(CC=C(C)C)COC(=O)C(F)(F)F
Mol. weight [g/mol]: 250.26

Physical Properties

Property code	Value	Unit	Source
hfus	24.23	kJ/mol	Joback Method
logp	3.640		Crippen Method
mcvol	184.090	ml/mol	McGowan Method
rinpol	1251.40		NIST Webbook
rinpol	1251.40		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.42	J/mol×K	544.99	Joback Method
cpg	467.85	J/mol×K	574.07	Joback Method
cpg	481.52	J/mol×K	603.16	Joback Method
cpg	494.47	J/mol×K	632.24	Joback Method
cpg	506.72	J/mol×K	661.32	Joback Method
cpg	518.31	J/mol×K	690.41	Joback Method
cpg	529.28	J/mol×K	719.49	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28673247&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices