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
CAS: 28673-24-7

Physical Properties

Property code	Value	Unit	Source
gf	-616.83	kJ/mol	Joback Method
hf	-915.10	kJ/mol	Joback Method
hfus	24.23	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.640		Crippen Method
mcvol	184.090	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1251.40		NIST Webbook
rinpol	1251.40		NIST Webbook
tb	544.99	K	Joback Method
tc	719.49	K	Joback Method
tf	251.59	K	Joback Method
vc	0.732	m3/kmol	Joback Method

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

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=C28673247&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