(.+/-.)-Lavandulol, methyl ether

Inchi: InChI=1S/C11H20O/c1-9(2)6-7-11(8-12-5)10(3)4/h6,11H,3,7-8H2,1-2,4-5H3
InchiKey: OEVGHYRSZABMFG-UHFFFAOYSA-N
Formula: C11H20O
SMILES: C=C(C)C(CC=C(C)C)COC
Mol. weight [g/mol]: 168.28

Physical Properties

Property code	Value	Unit	Source
gf	85.26	kJ/mol	Joback Method
hf	-184.80	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	41.55	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	3.181		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	1120.10		NIST Webbook
tb	473.66	K	Joback Method
tc	655.81	K	Joback Method
tf	186.20	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.14	J/mol×K	473.66	Joback Method
cpg	369.97	J/mol×K	504.02	Joback Method
cpg	385.11	J/mol×K	534.38	Joback Method
cpg	399.57	J/mol×K	564.74	Joback Method
cpg	413.38	J/mol×K	595.09	Joback Method
cpg	426.56	J/mol×K	625.45	Joback Method
cpg	439.13	J/mol×K	655.81	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=U352627&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume