«beta»-Cyclolavandulyl acetate

Inchi: InChI=1S/C12H20O2/c1-9-7-12(3,4)6-5-11(9)8-14-10(2)13/h5-8H2,1-4H3
InchiKey: PJBZKRBNXOKTOE-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC(=O)OCC1=C(C)CC(C)(C)CC1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-154.10	kJ/mol	Joback Method
hf	-431.41	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	52.36	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.076		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	1303.00		NIST Webbook
rinpol	1303.00		NIST Webbook
ripol	1655.00		NIST Webbook
tb	579.16	K	Joback Method
tc	790.19	K	Joback Method
tf	354.24	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.72	J/mol×K	579.16	Joback Method
cpg	450.99	J/mol×K	614.33	Joback Method
cpg	467.37	J/mol×K	649.50	Joback Method
cpg	482.95	J/mol×K	684.67	Joback Method
cpg	497.82	J/mol×K	719.85	Joback Method
cpg	512.06	J/mol×K	755.02	Joback Method
cpg	525.76	J/mol×K	790.19	Joback Method

Sources

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=R418818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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