Lilial

Other names:	Propanal, «alpha»-methyl-«beta»-(p-tert.-butylphenyl)- p-tert-Butyl-«alpha»-methylhydrocinnamaldehyde Benzenepropanal, 4-(1,1-dimethylethyl)-«alpha»-methyl- «alpha»-Methyl-p-(tert-butyl)hydrocinnamaldehyde «alpha»-Methyl, «beta»-(p-tert-butylphenyl)propionaldehyde p-tert-Butyl-«alpha»-methylhydrocinnamic aldehyde Hydrocinnamaldehyde, p-tert-butyl-«alpha»-methyl- Lilyal Propionaldehyde, «beta»-(4-tert-butylphenyl)-«alpha»-methyl- p-t-Butyl-«alpha»-methylhydrocinnamaldehyde Benzenepropanal, 4-tert-butyl-«alpha»-methyl- Lily aldehyde Benzenepropanal, 4-(tert-butyl)-alpha-methyl- 4-tert-butyl-«alpha»-methyl hydrocinnamic aldehyde 2-[(4-tert-Butylphenyl)methyl]propanal NSC 22275 2-(4-tert-butylbenzyl)propionaldehyde
Inchi:	InChI=1S/C14H20O/c1-11(10-15)9-12-5-7-13(8-6-12)14(2,3)4/h5-8,10-11H,9H2,1-4H3
InchiKey:	SDQFDHOLCGWZPU-UHFFFAOYSA-N
Formula:	C14H20O
SMILES:	CC(C=O)Cc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	204.31
CAS:	80-54-6

Physical Properties

Property code	Value	Unit	Source
gf	70.66	kJ/mol	Joback Method
hf	-206.84	kJ/mol	Joback Method
hfus	17.02	kJ/mol	Joback Method
hvap	54.73	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.362		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1535.00		NIST Webbook

rinpol	1500.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1549.00		NIST Webbook
tb	596.37	K	Joback Method
tc	810.62	K	Joback Method
tf	315.90	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.46	J/mol×K	596.37	Joback Method
cpg	487.89	J/mol×K	632.08	Joback Method
cpg	504.19	J/mol×K	667.79	Joback Method
cpg	519.42	J/mol×K	703.50	Joback Method
cpg	533.64	J/mol×K	739.20	Joback Method
cpg	546.93	J/mol×K	774.91	Joback Method
cpg	559.32	J/mol×K	810.62	Joback Method
dvisc	0.0038097	Pa×s	315.90	Joback Method
dvisc	0.0016292	Pa×s	362.65	Joback Method
dvisc	0.0008459	Pa×s	409.39	Joback Method
dvisc	0.0005023	Pa×s	456.13	Joback Method
dvisc	0.0003286	Pa×s	502.88	Joback Method
dvisc	0.0002311	Pa×s	549.62	Joback Method
dvisc	0.0001717	Pa×s	596.37	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=C80546&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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