Linalyl benzoate

Inchi: InChI=1S/C17H22O2/c1-5-17(4,13-9-10-14(2)3)19-16(18)15-11-7-6-8-12-15/h5-8,10-12H
InchiKey: BTJXBZZBBNNTOV-UHFFFAOYSA-N
Formula: C17H22O2
SMILES: C=CC(C)(CCC=C(C)C)OC(=O)c1ccccc1
Mol. weight [g/mol]: 258.36
CAS: 126-64-7

Physical Properties

Property code	Value	Unit	Source
gf	133.10	kJ/mol	Joback Method
hf	-178.37	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	62.94	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.535		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1781.00		NIST Webbook
rinpol	1780.80		NIST Webbook
tb	688.82	K	Joback Method
tc	905.47	K	Joback Method
tf	361.55	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.77	J/mol×K	688.82	Joback Method
cpg	628.09	J/mol×K	724.93	Joback Method
cpg	644.23	J/mol×K	761.04	Joback Method
cpg	659.29	J/mol×K	797.14	Joback Method
cpg	673.33	J/mol×K	833.25	Joback Method
cpg	686.45	J/mol×K	869.36	Joback Method
cpg	698.73	J/mol×K	905.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126647&Units=SI
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

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

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