sinensal

Other names: d-Sinensal
Inchi: InChI=1S/C15H22O/c1-5-13(2)8-6-9-14(3)10-7-11-15(4)12-16/h5,7-9,11-12,15H,1,6,10H
InchiKey: RXQNWMJVIQQHEU-XURCXITPSA-N
Formula: C15H22O
SMILES: C=CC(C)=CCC=C(C)CC=CC(C)C=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	284.86	kJ/mol	Joback Method
hf	13.72	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.236		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1696.00		NIST Webbook
rinpol	1696.00		NIST Webbook
ripol	2262.00		NIST Webbook
ripol	2262.00		NIST Webbook
tb	599.74	K	Joback Method
tc	794.51	K	Joback Method
tf	240.89	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.95	J/mol×K	599.74	Joback Method
cpg	526.43	J/mol×K	632.20	Joback Method
cpg	541.96	J/mol×K	664.66	Joback Method
cpg	556.63	J/mol×K	697.13	Joback Method
cpg	570.49	J/mol×K	729.59	Joback Method

cpg	583.61	J/mol×K	762.05	Joback Method
cpg	596.07	J/mol×K	794.51	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=R197249&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume