epi-Catalponol

Inchi: InChI=1S/C15H18O2/c1-10(2)7-8-11-9-14(16)12-5-3-4-6-13(12)15(11)17/h3-7,11,14,16H
InchiKey: BTQXIESSQVRLCV-ZSOXZCCMSA-N
Formula: C15H18O2
SMILES: CC(C)=CCC1CC(O)c2ccccc2C1=O
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	31.40	kJ/mol	Joback Method
hf	-264.07	kJ/mol	Joback Method
hfus	27.85	kJ/mol	Joback Method
hvap	72.66	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.279		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1988.00		NIST Webbook
tb	744.64	K	Joback Method
tc	965.00	K	Joback Method
tf	417.93	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.97	J/mol×K	744.64	Joback Method
cpg	574.45	J/mol×K	781.37	Joback Method
cpg	588.90	J/mol×K	818.09	Joback Method
cpg	602.35	J/mol×K	854.82	Joback Method
cpg	614.86	J/mol×K	891.54	Joback Method
cpg	626.48	J/mol×K	928.27	Joback Method
cpg	637.24	J/mol×K	965.00	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=R643311&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume