Amorpha-4,7-dien-11-ol

Inchi: InChI=1S/C15H24O/c1-10-5-7-12-11(2)6-8-14(13(12)9-10)15(3,4)16/h8-9,11-13,16H,5-7
InchiKey: NDCHPLODETXAFI-PNESKVBLSA-N
Formula: C15H24O
SMILES: CC1=CC2C(C(C)(C)O)=CCC(C)C2CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	47.49	kJ/mol	Joback Method
hf	-320.67	kJ/mol	Joback Method
hfus	21.89	kJ/mol	Joback Method
hvap	66.48	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1613.00		NIST Webbook
tb	665.72	K	Joback Method
tc	873.43	K	Joback Method
tf	366.17	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.61	J/mol×K	665.72	Joback Method
cpg	597.42	J/mol×K	700.34	Joback Method
cpg	615.05	J/mol×K	734.96	Joback Method
cpg	631.57	J/mol×K	769.57	Joback Method
cpg	647.05	J/mol×K	804.19	Joback Method
cpg	661.53	J/mol×K	838.81	Joback Method
cpg	675.10	J/mol×K	873.43	Joback Method
dvisc	0.0038419	Pa×s	366.17	Joback Method
dvisc	0.0014551	Pa×s	416.10	Joback Method

dvisc	0.0006785	Pa×s	466.02	Joback Method
dvisc	0.0003668	Pa×s	515.95	Joback Method
dvisc	0.0002210	Pa×s	565.87	Joback Method
dvisc	0.0001445	Pa×s	615.80	Joback Method
dvisc	0.0001007	Pa×s	665.72	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=R227048&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
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