Amorpha-4,9-dien-2-ol

Inchi: InChI=1S/C15H24O/c1-9(2)12-6-5-11(4)15-13(12)7-10(3)8-14(15)16/h5,7,9,12-16H,6,8H
InchiKey: STLBTFMCSOXEAQ-NAOUJUTFSA-N
Formula: C15H24O
SMILES: CC1=CC2C(C(C)C)CC=C(C)C2C(O)C1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	34.50	kJ/mol	Joback Method
hf	-337.54	kJ/mol	Joback Method
hfus	26.85	kJ/mol	Joback Method
hvap	67.08	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.552		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1687.00		NIST Webbook
tb	663.84	K	Joback Method
tc	864.81	K	Joback Method
tf	344.51	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.38	J/mol×K	663.84	Joback Method
cpg	662.51	J/mol×K	831.32	Joback Method
cpg	647.70	J/mol×K	797.82	Joback Method
cpg	631.91	J/mol×K	764.33	Joback Method
cpg	615.12	J/mol×K	730.83	Joback Method
cpg	597.29	J/mol×K	697.34	Joback Method
cpg	676.39	J/mol×K	864.81	Joback Method
dvisc	0.0001311	Pa×s	663.84	Joback Method

dvisc	0.0001823	Pa×s	610.62	Joback Method
dvisc	0.0002700	Pa×s	557.40	Joback Method
dvisc	0.0004346	Pa×s	504.17	Joback Method
dvisc	0.0007826	Pa×s	450.95	Joback Method
dvisc	0.0016494	Pa×s	397.73	Joback Method
dvisc	0.0043769	Pa×s	344.51	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=R281626&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