Amorpha-2,4,7(11)-triene

Other names: (+)-(1S,6S,10S)-Amorpha-2,4,7(11)-triene
Inchi: InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,7,9,12,14-15H,6,8H2,
InchiKey: QNFAKPNPKWLYEY-CFVMTHIKSA-N
Formula: C15H22
SMILES: CC1=CC2C(=C(C)C)CCC(C)C2C=C1
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	228.01	kJ/mol	Joback Method
hf	-81.98	kJ/mol	Joback Method
hfus	24.62	kJ/mol	Joback Method
hvap	51.30	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.501		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
tb	578.31	K	Joback Method
tc	798.74	K	Joback Method
tf	286.81	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.35	J/mol×K	578.31	Joback Method
cpg	505.27	J/mol×K	615.05	Joback Method
cpg	525.87	J/mol×K	651.79	Joback Method
cpg	545.20	J/mol×K	688.53	Joback Method
cpg	563.31	J/mol×K	725.27	Joback Method
cpg	580.28	J/mol×K	762.00	Joback Method

cpg	596.16	J/mol×K	798.74	Joback Method

Sources

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=R427095&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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