(-)-(1R,6S,10S)-Amorpha-4,7(11)-dien-3-one

Inchi: InChI=1S/C15H22O/c1-9(2)12-6-5-10(3)13-8-15(16)11(4)7-14(12)13/h7,10,13-14H,5-6,8
InchiKey: WCBCKXJLRYPWHZ-LEWSCRJBSA-N
Formula: C15H22O
SMILES: CC1=CC2C(=C(C)C)CCC(C)C2CC1=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	75.46	kJ/mol	Joback Method
hf	-277.46	kJ/mol	Joback Method
hfus	22.90	kJ/mol	Joback Method
hvap	55.26	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
tb	646.97	K	Joback Method
tc	877.91	K	Joback Method
tf	354.27	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.31	J/mol×K	646.97	Joback Method
cpg	566.22	J/mol×K	685.46	Joback Method
cpg	586.78	J/mol×K	723.95	Joback Method
cpg	606.00	J/mol×K	762.44	Joback Method
cpg	623.93	J/mol×K	800.93	Joback Method
cpg	640.58	J/mol×K	839.42	Joback Method
cpg	655.99	J/mol×K	877.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515865&Units=SI
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

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