

Amorpha-4,9-dien-14-al

Inchi:	InChI=1S/C15H22O/c1-10(2)13-6-4-11(3)14-7-5-12(9-16)8-15(13)14/h4,8-10,13-15H,5-7
InchiKey:	XOJRZWAZKRAFFU-WLYUNCDWSA-N
Formula:	C15H22O
SMILES:	CC1=CCC(C(C)C)C2C=C(C=O)CCC12
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
gf	79.51	kJ/mol	Joback Method
hf	-250.55	kJ/mol	Joback Method
hfus	23.98	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.760		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinsol	1692.00		NIST Webbook
rinsol	1692.00		NIST Webbook
tb	624.99	K	Joback Method
tc	842.80	K	Joback Method
tf	329.93	K	Joback Method
vc	0.740	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.53	J/mol×K	624.99	Joback Method
cpg	552.07	J/mol×K	661.29	Joback Method
cpg	571.34	J/mol×K	697.59	Joback Method
cpg	589.38	J/mol×K	733.89	Joback Method
cpg	606.26	J/mol×K	770.20	Joback Method
cpg	622.01	J/mol×K	806.50	Joback Method
cpg	636.68	J/mol×K	842.80	Joback Method
dvisc	0.0025245	Paxs	329.93	Joback Method

dvisc	0.0015545	Paxs	379.11	Joback Method
dvisc	0.0010699	Paxs	428.28	Joback Method
dvisc	0.0007953	Paxs	477.46	Joback Method
dvisc	0.0006249	Paxs	526.64	Joback Method
dvisc	0.0005116	Paxs	575.81	Joback Method
dvisc	0.0004322	Paxs	624.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R281611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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