

Acora-3,5-diene-11-ol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24O/c1-11-7-9-15(10-8-11)12(2)5-6-13(15)14(3,4)16/h7-9,12-13,16H,5-6

AQVXTKFYDNDQTE-UHFFFAOYSA-N

C15H24O

CC1=CCC2(C=C1)C(C)CCC2C(C)(C)O

220.35

Physical Properties

Property code	Value	Unit	Source
gf	51.63	kJ/mol	Joback Method
hf	-293.96	kJ/mol	Joback Method
hfus	15.98	kJ/mol	Joback Method
hvap	64.67	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1568.00		NIST Webbook
rinpol	1568.00		NIST Webbook
tb	660.98	K	Joback Method
tc	875.00	K	Joback Method
tf	377.55	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.18	J/mol×K	660.98	Joback Method
cpg	594.14	J/mol×K	696.65	Joback Method
cpg	612.03	J/mol×K	732.32	Joback Method
cpg	629.01	J/mol×K	767.99	Joback Method
cpg	645.25	J/mol×K	803.66	Joback Method
cpg	660.89	J/mol×K	839.33	Joback Method
cpg	676.10	J/mol×K	875.00	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=R203839&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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