

(1R,5R)-1-Isopropyl-8-methyl-4-methylenespiro[4.5]

Other names:	Spiro[4.5]dec-7-ene, 8-methyl-1-methylene-4-(1-methylethyl)-, (4R,5R)- Spiro[4.5]dec-7-ene, 8-methyl-1-methylene-4-(1-methylethyl)-, (4R-trans)- (+)-Acora-3,7(14)-diene Acora-3(7),14-diene
Inchi:	InChI=1S/C15H24/c1-11(2)14-6-5-13(4)15(14)9-7-12(3)8-10-15/h7,11,14H,4-6,8-10H2,1
InchiKey:	QZGRYPDXCBFNRS-GJZGRUSLSA-N
Formula:	C15H24
SMILES:	C=C1CCC(C(C)C)C12CC=C(C)CC2
Mol. weight [g/mol]:	204.35
CAS:	55732-78-0

Physical Properties

Property code	Value	Unit	Source
gf	214.00	kJ/mol	Joback Method
hf	-91.46	kJ/mol	Joback Method
hfus	12.33	kJ/mol	Joback Method
hvap	49.07	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1408.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1404.00		NIST Webbook
tb	576.26	K	Joback Method
tc	799.10	K	Joback Method
tf	316.47	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.60	J/mol×K	576.26	Joback Method

cpg	522.01	J/mol×K	613.40	Joback Method
cpg	543.03	J/mol×K	650.54	Joback Method
cpg	562.83	J/mol×K	687.68	Joback Method
cpg	581.54	J/mol×K	724.82	Joback Method
cpg	599.33	J/mol×K	761.96	Joback Method
cpg	616.34	J/mol×K	799.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55732780&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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