

Spiro[5.5]undeca-1,8-diene, 1,5,5,9-tetramethyl-, (R)-

Other names:	«alpha»-Chamigrene Spiro[5.5]undeca-1,8-diene, 1,5,5,9-tetramethyl-
Inchi:	InChI=1S/C15H24/c1-12-7-10-15(11-8-12)13(2)6-5-9-14(15,3)4/h6-7H,5,8-11H2,1-4H3
InchiKey:	SIBCECUUMHIAAM-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1=CCC2(CC1)C(C)=CCCC2(C)C
Mol. weight [g/mol]:	204.35
CAS:	19912-83-5

Physical Properties

Property code	Value	Unit	Source
gf	166.10	kJ/mol	Joback Method
hf	-115.03	kJ/mol	Joback Method
hfus	9.45	kJ/mol	Joback Method
hvap	49.28	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1514.20		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1523.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1753.00		NIST Webbook
tb	586.19	K	Joback Method
tc	822.53	K	Joback Method
tf	351.45	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.78	J/mol×K	586.19	Joback Method
cpg	523.43	J/mol×K	625.58	Joback Method
cpg	544.65	J/mol×K	664.97	Joback Method
cpg	564.73	J/mol×K	704.36	Joback Method
cpg	583.94	J/mol×K	743.75	Joback Method
cpg	602.58	J/mol×K	783.14	Joback Method
cpg	620.93	J/mol×K	822.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19912835&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
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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