Spiro[5.5]undec-2-ene, 3,7,7-trimethyl-11-methylene-, (-)-

Other names:	«beta»-Chamigrene
	Chamigren
	Chamigrene
	Spiro[5.5]undec-2-ene, 3,7,7-trimethyl-11-methylene-, (R)-
Inchi:	InChI=1S/C15H24/c1-12-7-10-15(11-8-12)13(2)6-5-9-14(15,3)4/h7H,2,5-6,8-11H2,1,3-4H
InchiKey:	WLNGPDPILFYWKF-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C1CCCC(C)(C)C12CC=C(C)CC2
Mol. weight [g/mol]:	204.35
CAS:	18431-82-8

Physical Properties

Property code	Value	Unit	Source
gf	198.85	kJ/mol	Joback Method
hf	-77.10	kJ/mol	Joback Method
hfus	7.45	kJ/mol	Joback Method
hvap	48.48	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1495.00		NIST Webbook

rinpol	1478.00	NIST Webbook
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rinpol	1451.00	NIST Webbook
rinpol	1474.00	NIST Webbook
rinpol	1503.00	NIST Webbook
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rinpol	1473.00		NIST Webbook
ripol	1735.00		NIST Webbook
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ripol	1724.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1755.00		NIST Webbook
tb	581.21	K	Joback Method
tc	816.28	K	Joback Method
tf	351.85	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.46	J/mol×K	581.21	Joback Method
cpg	522.35	J/mol×K	620.39	Joback Method
cpg	543.78	J/mol×K	659.57	Joback Method
cpg	564.03	J/mol×K	698.74	Joback Method
cpg	583.37	J/mol×K	737.92	Joback Method
cpg	602.08	J/mol×K	777.10	Joback Method
cpg	620.44	J/mol×K	816.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18431828&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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