(1R,9R,E)-4,11,11-Trimethyl-8-methylenebicyclo[7

Other names: Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, (1R,4E,9R)-
Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9R*)]-
(+)-9-epi-«beta»-Caryophyllene
9-epi-(E)-Caryophyllene
9-epi-trans-Caryophyllene
9-epi-«beta»-Caryophyllene
epi-«beta»-Caryophyllene
9-epi-(E)-Caryophillene

Inchi: InChI=1S/C15H24/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/h6,13-14H,2,5,7-10H2,1,

InchiKey: NPNUFJAVOOONJE-BLOBHPOZSA-N

Formula: C15H24

SMILES: C=C1CCC=C(C)CCC2C1CC2(C)C

Mol. weight [g/mol]: 204.35

CAS: 68832-35-9

Physical Properties

Property code	Value	Unit	Source
gf	196.63	kJ/mol	Joback Method
hf	-112.68	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1465.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1467.00		NIST Webbook

rinpol	1466.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1471.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1572.00		NIST Webbook
ripol	1563.00		NIST Webbook
tb	576.30	K	Joback Method
tc	802.06	K	Joback Method
tf	323.71	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.77	J/mol×K	576.30	Joback Method
cpg	525.28	J/mol×K	613.93	Joback Method
cpg	547.37	J/mol×K	651.55	Joback Method
cpg	568.18	J/mol×K	689.18	Joback Method
cpg	587.84	J/mol×K	726.81	Joback Method
cpg	606.51	J/mol×K	764.43	Joback Method
cpg	624.31	J/mol×K	802.06	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=C68832359&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