Bicyclo[2.2.1]heptane, 2-methyl-3-methylene-2-(4-methyl-3-pentenyl)-, (1S-exo)-

Other names: Norbornane, 2-methyl-3-methylene-2-(4-methyl-3-pentenyl)-
«beta»-Santalene
(-)-«beta»-Santalene
(1S-exo)-2-methyl-3-methylene-2-(4-methyl-3-pentenyl)bicyclo[2.2.1]heptane

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

InchiKey: PGBNIHXXFQBCPU-NRXISQOPSA-N

Formula: C15H24

SMILES: C=C1C2CCC(C2)C1(C)CCC=C(C)C

Mol. weight [g/mol]: 204.35

CAS: 511-59-1

Physical Properties

Property code	Value	Unit	Source
gf	296.37	kJ/mol	Joback Method
hf	-26.92	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1461.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1437.00		NIST Webbook

rinpol	1463.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1463.30		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1653.00		NIST Webbook
tb	559.12	K	Joback Method
tc	765.28	K	Joback Method
tf	305.47	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.48	J/mol×K	559.12	Joback Method
cpg	516.19	J/mol×K	593.48	Joback Method
cpg	535.61	J/mol×K	627.84	Joback Method
cpg	553.91	J/mol×K	662.20	Joback Method
cpg	571.23	J/mol×K	696.56	Joback Method
cpg	587.73	J/mol×K	730.92	Joback Method
cpg	603.56	J/mol×K	765.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C511591&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
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