Tricyclo[2.2.1.0(2,6)]heptane, 1,7-dimethyl-7-(4-methyl-3-pentenyl)-, (-)-

Other names: «alpha»-Santalene
(-)-«alpha»-Santalene
Santalen
Santalene
1,7-Dimethyl-7-(4-methyl-3-pentenyl)-tricyclo[2.2.1.0(2,6)]heptane, (-)-
1,7-Dimethyl-7-(4-methyl-3-pentenyl)-tricyclo[2.2.1.0(2,6)]heptane

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

InchiKey: KWFJIXPIFLVMPM-UHFFFAOYSA-N

Formula: C15H24

SMILES: CC(C)=CCCC1(C)C2CC3C(C2)C31C

Mol. weight [g/mol]: 204.35

CAS: 512-61-8

Physical Properties

Property code	Value	Unit	Source
gf	327.14	kJ/mol	Joback Method
hf	-24.98	kJ/mol	Joback Method
hfus	21.65	kJ/mol	Joback Method
hvap	45.50	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1420.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1424.20		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1421.00		NIST Webbook

rinpol	1428.00	NIST Webbook
rinpol	1418.00	NIST Webbook
rinpol	1428.00	NIST Webbook
rinpol	1440.00	NIST Webbook
rinpol	1414.00	NIST Webbook
rinpol	1435.00	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1421.00	NIST Webbook
rinpol	1412.00	NIST Webbook
rinpol	1428.00	NIST Webbook
rinpol	1432.00	NIST Webbook
rinpol	1405.00	NIST Webbook
rinpol	1405.00	NIST Webbook
rinpol	1407.00	NIST Webbook
rinpol	1409.00	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1412.00	NIST Webbook
rinpol	1412.00	NIST Webbook
rinpol	1418.00	NIST Webbook
rinpol	1415.00	NIST Webbook
rinpol	1423.00	NIST Webbook
rinpol	1414.00	NIST Webbook
rinpol	1414.00	NIST Webbook
rinpol	1418.00	NIST Webbook
rinpol	1412.00	NIST Webbook
rinpol	1410.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1412.00	NIST Webbook
rinpol	1412.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1418.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1470.00	NIST Webbook
rinpol	1420.00	NIST Webbook
rinpol	1409.00	NIST Webbook
ripol	1566.00	NIST Webbook
ripol	1601.00	NIST Webbook
ripol	1555.00	NIST Webbook
ripol	1574.00	NIST Webbook
ripol	1574.00	NIST Webbook
ripol	1574.00	NIST Webbook
ripol	1583.00	NIST Webbook
ripol	1597.00	NIST Webbook

ripol	1608.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1576.00		NIST Webbook
tb	549.46	K	Joback Method
tc	755.18	K	Joback Method
tf	339.95	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.79	J/mol×K	549.46	Joback Method
cpg	518.15	J/mol×K	583.75	Joback Method
cpg	537.02	J/mol×K	618.03	Joback Method
cpg	554.67	J/mol×K	652.32	Joback Method
cpg	571.36	J/mol×K	686.61	Joback Method
cpg	587.36	J/mol×K	720.90	Joback Method
cpg	602.95	J/mol×K	755.18	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C512618&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

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