7-epi-«alpha»-Selinene

Other names: 7 epi-a-Selinene
Inchi: InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h6,13-14H,1,5,7-10H2,2-
InchiKey: OZQAPQSEYFAMCY-UHFFFAOYSA-N
Formula: C15H24
SMILES: C=C(C)C1CCC2(C)CCC=C(C)C2C1
Mol. weight [g/mol]: 204.35
CAS: 123123-37-5

Physical Properties

Property code	Value	Unit	Source
gf	234.94	kJ/mol	Joback Method
hf	-75.12	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1517.00		NIST Webbook

rinpol	1517.00	NIST Webbook
rinpol	1503.00	NIST Webbook
rinpol	1516.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1540.00	NIST Webbook
rinpol	1518.00	NIST Webbook
rinpol	1511.00	NIST Webbook
rinpol	1524.00	NIST Webbook
rinpol	1523.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1517.00	NIST Webbook
rinpol	1524.80	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1513.00	NIST Webbook
rinpol	1522.00	NIST Webbook
rinpol	1512.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1517.00	NIST Webbook
rinpol	1519.00	NIST Webbook
rinpol	1524.00	NIST Webbook
rinpol	1548.00	NIST Webbook
rinpol	1515.00	NIST Webbook
rinpol	1514.00	NIST Webbook
rinpol	1494.00	NIST Webbook
rinpol	1506.00	NIST Webbook
rinpol	1486.00	NIST Webbook
rinpol	1511.00	NIST Webbook
rinpol	1518.00	NIST Webbook
rinpol	1508.00	NIST Webbook
rinpol	1470.00	NIST Webbook
rinpol	1516.00	NIST Webbook
rinpol	1517.00	NIST Webbook
rinpol	1492.00	NIST Webbook
rinpol	1518.00	NIST Webbook
rinpol	1527.00	NIST Webbook
rinpol	1526.00	NIST Webbook
rinpol	1516.00	NIST Webbook
rinpol	1534.00	NIST Webbook
rinpol	1530.00	NIST Webbook
rinpol	1514.00	NIST Webbook
ripol	1754.00	NIST Webbook
ripol	1762.00	NIST Webbook

ripol	1758.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1772.00		NIST Webbook
tb	569.43	K	Joback Method
tc	794.31	K	Joback Method
tf	297.83	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.65	J/mol×K	569.43	Joback Method
cpg	523.17	J/mol×K	606.91	Joback Method
cpg	545.19	J/mol×K	644.39	Joback Method
cpg	565.88	J/mol×K	681.87	Joback Method
cpg	585.40	J/mol×K	719.35	Joback Method
cpg	603.90	J/mol×K	756.83	Joback Method
cpg	621.57	J/mol×K	794.31	Joback Method

Sources

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=C123123375&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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