

«delta»-Selinene

Inchi:	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h10-11H,5-9H2,1-4H3
InchiKey:	VEGYMPQCXPVQJY-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1=C2C=C(C(C)C)CCC2(C)CCC1
Mol. weight [g/mol]:	204.35
CAS:	28624-23-9

Physical Properties

Property code	Value	Unit	Source
gf	179.33	kJ/mol	Joback Method
hf	-120.52	kJ/mol	Joback Method
hfus	12.86	kJ/mol	Joback Method
hvap	50.84	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1479.00		NIST Webbook

rinpol	1483.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1501.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1707.00		NIST Webbook
ripol	1728.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1728.00		NIST Webbook
tb	590.89	K	Joback Method
tc	815.98	K	Joback Method
tf	332.83	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.51	J/mol×K	590.89	Joback Method
cpg	521.85	J/mol×K	628.41	Joback Method
cpg	541.90	J/mol×K	665.92	Joback Method
cpg	560.83	J/mol×K	703.44	Joback Method
cpg	578.78	J/mol×K	740.95	Joback Method
cpg	595.93	J/mol×K	778.47	Joback Method
cpg	612.42	J/mol×K	815.98	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=C28624239&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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