«beta»-Longipinene

Inchi: InChI=1S/C14H22/c1-9-6-7-11-10-5-4-8-14(2,3)13(11)12(9)10/h10-13H,1,4-8H2,2-3H3
InchiKey: VJRRUPHSDRBMPP-UHFFFAOYSA-N
Formula: C14H22
SMILES: C=C1CCC2C3CCCC(C)(C)C2C13
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	257.22	kJ/mol	Joback Method
hf	-67.41	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	45.23	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.025		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1432.50		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1396.00		NIST Webbook

rinpol	1418.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1403.20		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1398.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1599.00		NIST Webbook
tb	538.54	K	Joback Method
tc	757.73	K	Joback Method
tf	323.42	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.99	J/mol×K	538.54	Joback Method
cpg	474.07	J/mol×K	575.07	Joback Method
cpg	495.58	J/mol×K	611.60	Joback Method
cpg	515.69	J/mol×K	648.14	Joback Method
cpg	534.59	J/mol×K	684.67	Joback Method
cpg	552.44	J/mol×K	721.20	Joback Method
cpg	569.43	J/mol×K	757.73	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=R127547&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