cis-«beta»-santalene

Other names: (Z)-«beta»-santalene
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-ILXRZTDVSA-N
Formula: C15H24
SMILES: C=C1C2CCC(C2)C1(C)CCC=C(C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hf	-59.62	kJ/mol	Cheméo Relay (1.0)
hfus	21.28	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Cheméo Relay (1.0)
ie	8.28	eV	Cheméo Relay (1.0)
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1449.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1446.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1617.00		NIST Webbook
tb	538.70	K	Cheméo Relay (1.0)
tf	311.79	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R276283&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point