cis-(-)-2,4a,5,6,9a-Hexahydro-3,5,5,9-tetramethyl(1

Other names: 1H-Benzocycloheptene, 2,4a,5,6,9a-hexahydro-3,5,5,9-tetramethyl-, deriv.
Inchi: InChI=1S/C15H24/c1-11-7-8-13-12(2)6-5-9-15(3,4)14(13)10-11/h5-6,10,12-14H,7-9H2,1-
InchiKey: ARHRNUWNRNFXBZ-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1=CC2C(CC1)C(C)C=CCC2(C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	165.80	kJ/mol	Joback Method
hf	-159.48	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	49.15	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1478.00		NIST Webbook
tb	571.63	K	Joback Method
tc	797.59	K	Joback Method
tf	306.55	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.21	J/mol×K	571.63	Joback Method
cpg	527.37	J/mol×K	609.29	Joback Method
cpg	550.04	J/mol×K	646.95	Joback Method
cpg	571.38	J/mol×K	684.61	Joback Method
cpg	591.51	J/mol×K	722.27	Joback Method
cpg	610.58	J/mol×K	759.93	Joback Method

cpg	628.74	J/mol×K	797.59	Joback Method

Sources

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=U104201&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume