1H-Cyclopropa[a]naphthalene, 1a,2,3,3a,4,5,6,7b-octahydro-1,1,3a,7-tetramethyl-, [1aR-(1a«alpha»,3a«alpha», 7b«alpha»)]-

Other names: 1H-Cyclopropa[a]naphthalene, 1a,2,3,3a,4,5,6,7b-octahydro-1,1,3a,7-tetramethyl-, (1aR,3aS,7bS)-1,1,3a,7-Tetramethyl-1a,2,3,3a,4,5,6,7b-octahydro-1H-cyclopropa[a]naphthalene, «beta»-Maaliene

Inchi: InChI=1S/C15H24/c1-10-6-5-8-15(4)9-7-11-13(12(10)15)14(11,2)3/h11,13H,5-9H2,1-4H3

InchiKey: UPGLJTCDRBIZKP-UHFFFAOYSA-N

Formula: C15H24

SMILES: CC1=C2C3C(CCC2(C)CCC1)C3(C)C

Mol. weight [g/mol]: 204.35

CAS: 489-29-2

Physical Properties

Property code	Value	Unit	Source
gf	225.48	kJ/mol	Joback Method
hf	-101.87	kJ/mol	Joback Method
hfus	13.73	kJ/mol	Joback Method
hvap	48.07	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1418.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1413.70		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1417.00		NIST Webbook
ripol	1671.00		NIST Webbook
tb	576.29	K	Joback Method

tc	802.89	K	Joback Method
tf	374.95	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.46	J/mol×K	576.29	Joback Method
cpg	525.54	J/mol×K	614.06	Joback Method
cpg	546.15	J/mol×K	651.82	Joback Method
cpg	565.60	J/mol×K	689.59	Joback Method
cpg	584.18	J/mol×K	727.36	Joback Method
cpg	602.19	J/mol×K	765.12	Joback Method
cpg	619.93	J/mol×K	802.89	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=C489292&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