1,3a-Ethano-3aH-indene, 1,2,3,6,7,7a-hexahydro-2,2,4,7a-tetramethyl-, [1R-(1«alpha»,3a«alpha»,7a«alpha»)]-

Other names: Neoclovene
(-)-«alpha»-Neoclovene
«alpha»-Neoclovene

Inchi: InChI=1S/C15H24/c1-11-6-5-8-14(4)12-7-9-15(11,14)10-13(12,2)3/h6,12H,5,7-10H2,1-4

InchiKey: ZCJQJJWNFDNQGZ-HNFVBEJKSA-N

Formula: C15H24

SMILES: CC1=CCCC2(C)C3CCC12CC3(C)C

Mol. weight [g/mol]: 204.35

CAS: 4545-68-0

Physical Properties

Property code	Value	Unit	Source
gf	229.62	kJ/mol	Joback Method
hf	-75.16	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1466.50		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1453.00		NIST Webbook
ripol	1747.00		NIST Webbook

tb	571.55	K	Joback Method
tc	806.48	K	Joback Method
tf	386.33	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.53	J/mol×K	571.55	Joback Method
cpg	523.86	J/mol×K	610.71	Joback Method
cpg	544.56	J/mol×K	649.86	Joback Method
cpg	564.09	J/mol×K	689.02	Joback Method
cpg	582.88	J/mol×K	728.17	Joback Method
cpg	601.40	J/mol×K	767.33	Joback Method
cpg	620.08	J/mol×K	806.48	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=C4545680&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