

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

Other names: 1H-Cyclopropa[a]naphthalene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, [1aR,7R,7aR,7bS]-1,1,7,7a-Tetramethyl-1a,2,3,5,6,7,7a,7b-octahydro-1H-cyclopropa[a]naphthalene
«beta»-Gurjunene
«delta»1(10)-Aristolene
Calarene
1(10)-Aristolene, (+)-
(+)-Calarene
«delta»-Aristol-1(10)-ene
(+)-1(10)-Aristolene
(+)-«delta»1(10)-Aristolene
1(10)-Aristolene
«beta»-Gurjenene
Calarene (= «beta»-gurjunene)
«beta»-Gurjurene
Calarene («beta»-gurjunene)
«beta»-Gurjunene (calarene)
[1aR-(1a«alpha»,7«alpha»,7a«alpha»,7b«alpha»)]-1a,2,3,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-1H-cyclopropa[a]naphthalene
Inchi: InChI=1S/C15H24/c1-10-6-5-7-11-8-9-12-13(14(12,2)3)15(10,11)4/h7,10,12-13H,5-6,8-9H
InchiKey: MBIPADCEHSKJDQ-ADBWKJQBSA-N
Formula: C15H24
SMILES: CC1CCC=C2CCC3C(C3(C)C)C21C
Mol. weight [g/mol]: 204.35
CAS: 17334-55-3

Physical Properties

Property code	Value	Unit	Source
gf	227.40	kJ/mol	Joback Method
hf	-110.74	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	47.10	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
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tb	566.64	K	Joback Method
tc	792.17	K	Joback Method
tf	358.19	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.55	J/mol×K	566.64	Joback Method
cpg	526.55	J/mol×K	604.23	Joback Method
cpg	547.97	J/mol×K	641.82	Joback Method
cpg	568.10	J/mol×K	679.41	Joback Method
cpg	587.25	J/mol×K	716.99	Joback Method
cpg	605.70	J/mol×K	754.58	Joback Method
cpg	623.74	J/mol×K	792.17	Joback Method

Sources

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=C17334553&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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