

(1S,1aS,1bR,4S,5S,5aS,6aR)-1a,1b,4,5a-Tetramethy

Other names:	1,5-Methanocycloprop[a]indene, decahydro-1a,1b,4,5a-tetramethyl-, (1S,1aS,1bR,4S,5S,5aS,6aR)- 1,5-Methanocycloprop[a]indene, decahydro-1a,1b,4,5a-tetramethyl-, [1S-(1«alpha»,1a«beta»,1b«beta»,4«alpha»,5«alpha»,5a«beta»,6a«beta»)]- (-)-Cycloseychellene Cycloseychellene
Inchi:	InChI=1S/C15H24/c1-9-5-6-14(3)13(2)8-12-11(7-10(9)13)15(12,14)4/h9-12H,5-8H2,1-4H
InchiKey:	XPWRIXBORAHMCD-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1CCC2(C)C3(C)CC4C(CC13)C42C
Mol. weight [g/mol]:	204.35
CAS:	52617-34-2

Physical Properties

Property code	Value	Unit	Source
gf	290.92	kJ/mol	Joback Method
hf	-70.87	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	44.08	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	4.105		Crippen Method
mcvol	178.770	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1417.90		NIST Webbook
rinpol	1417.90		NIST Webbook
tb	552.00	K	Joback Method
tc	775.96	K	Joback Method
tf	393.07	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.97	J/mol×K	552.00	Joback Method
cpg	526.89	J/mol×K	589.33	Joback Method
cpg	547.94	J/mol×K	626.65	Joback Method

cpg	567.56	J/mol×K	663.98	Joback Method
cpg	586.20	J/mol×K	701.31	Joback Method
cpg	604.29	J/mol×K	738.63	Joback Method
cpg	622.26	J/mol×K	775.96	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=C52617342&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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