

(3aS,8aS)-6,8a-Dimethyl-3-(propan-2-ylidene)-1,2,3,4,5,6,7,8a-octahydro-1H-indene

Inchi:	InChI=1S/C15H24/c1-11(2)13-8-10-15(4)9-7-12(3)5-6-14(13)15/h7,14H,5-6,8-10H2,1-4H3
InchiKey:	PRQLWQYYMJZORK-GJZGRUSLSA-N
Formula:	C15H24
SMILES:	CC1=CCC2(C)CCC(=C(C)C)C2CC1
Mol. weight [g/mol]:	204.35
CAS:	395070-76-5

Physical Properties

Property code	Value	Unit	Source
gf	200.27	kJ/mol	Joback Method
hf	-104.18	kJ/mol	Joback Method
hfus	16.02	kJ/mol	Joback Method
hvap	50.17	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1532.20		NIST Webbook
tb	584.06	K	Joback Method
tc	811.24	K	Joback Method
tf	314.19	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.06	J/mol×K	584.06	Joback Method
cpg	523.47	J/mol×K	621.92	Joback Method
cpg	544.48	J/mol×K	659.79	Joback Method
cpg	564.25	J/mol×K	697.65	Joback Method
cpg	582.97	J/mol×K	735.51	Joback Method
cpg	600.80	J/mol×K	773.38	Joback Method
cpg	617.92	J/mol×K	811.24	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=C395070765&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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