

1,1,4-Trimethyl-7-methylene-1a,2,3,5,6,7,7a,7b-oct

Inchi:	InChI=1S/C15H22/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h12-14H,2,5-8H2,1,3-4
InchiKey:	OBPkUBNSEKJPHY-HPNrgHHYSA-N
Formula:	C15H22
SMILES:	<chem>C=C1CCC2=C(C)CCC3C(C12)C3(C)C</chem>
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	284.05	kJ/mol	Joback Method
hf	-32.87	kJ/mol	Joback Method
hfus	18.87	kJ/mol	Joback Method
hvap	49.38	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinsol	1510.00		NIST Webbook
tb	575.21	K	Joback Method
tc	794.86	K	Joback Method
tf	364.73	K	Joback Method
vc	0.698	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.12	J/mol×K	575.21	Joback Method
cpg	505.10	J/mol×K	611.82	Joback Method
cpg	524.76	J/mol×K	648.43	Joback Method
cpg	543.26	J/mol×K	685.04	Joback Method
cpg	560.79	J/mol×K	721.65	Joback Method
cpg	577.52	J/mol×K	758.25	Joback Method
cpg	593.62	J/mol×K	794.86	Joback Method

Sources

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=R407724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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