

1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis-

Other names: 1H-Benzocyclohepten-7-ol,
2,3,4,4a,5,6,7,8-octahydro-1,1,4a«alpha»,7«beta»-tetramethyl-
widrol

Inchi: InChI=1S/C15H26O/c1-13(2)7-5-8-14(3)10-11-15(4,16)9-6-12(13)14/h6,16H,5,7-11H2,1-4H

InchiKey: BXGVVQADPFXGHD-LOACHALJSA-N

Formula: C15H26O

SMILES: CC1(O)CC=C2C(C)(C)CCCC2(C)CC1

Mol. weight [g/mol]: 222.37

CAS: 6892-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-4.25	kJ/mol	Joback Method
hf	-318.67	kJ/mol	Joback Method
hfus	7.47	kJ/mol	Joback Method
hvap	63.54	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.064		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1587.00		NIST Webbook
rinpol	1587.00		NIST Webbook
rinpol	1616.60		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1587.00		NIST Webbook
ripol	2179.00		NIST Webbook

ripol	2179.00		NIST Webbook
ripol	2178.00		NIST Webbook
tb	669.80	K	Joback Method
tc	892.10	K	Joback Method
tf	418.65	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.96	J/mol×K	669.80	Joback Method
cpg	610.99	J/mol×K	706.85	Joback Method
cpg	630.41	J/mol×K	743.90	Joback Method
cpg	649.54	J/mol×K	780.95	Joback Method
cpg	668.73	J/mol×K	818.00	Joback Method
cpg	688.28	J/mol×K	855.05	Joback Method
cpg	708.53	J/mol×K	892.10	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=C6892804&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

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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