2H-2,4a-Methanonaphthalen-8(5H)-one, 1,3,4,6,7,8a-hexahydro-1,1,5,5-tetramethyl-

Other names: 2H-2,4a-Methanonaphthalen-8(5H)-one, hexahydro-1,1,5,5-tetramethyl-
trans-Isolongifolanone
cis-Isolongifolanone
Isolongifolanone, trans- (piconia)
1,3,4,6,7,8a-hexahydro-1,1,5,5-tetramethyl-2H-2,4a-methanonaphthalen-8(5H)-one

Inchi: InChI=1S/C15H24O/c1-13(2)7-6-11(16)12-14(3,4)10-5-8-15(12,13)9-10/h10,12H,5-9H2,1

InchiKey: VCOCESNMLNDPLX-UHFFFAOYSA-N

Formula: C15H24O

SMILES: CC1(C)C2CCC3(C2)C1C(=O)CCC3(C)C

Mol. weight [g/mol]: 220.35

CAS: 23787-90-8

Physical Properties

Property code	Value	Unit	Source
gf	78.99	kJ/mol	Joback Method
hf	-279.51	kJ/mol	Joback Method
hfus	7.57	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.818		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	630.56	K	Joback Method
tc	875.45	K	Joback Method
tf	437.03	K	Joback Method

vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.94	J/mol×K	630.56	Joback Method
cpg	584.99	J/mol×K	671.37	Joback Method
cpg	606.96	J/mol×K	712.19	Joback Method
cpg	628.30	J/mol×K	753.00	Joback Method
cpg	649.46	J/mol×K	793.82	Joback Method
cpg	670.93	J/mol×K	834.63	Joback Method
cpg	693.14	J/mol×K	875.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23787908&Units=SI
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

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