1,4:5,8-Dimethanonaphthalen-9-one, 1,4,4a,5,6,7,8,8a-octahydro-, (1α,4α,4aα,5&#946,8β,8a&#

Other names: 1,4:5,8-Dimethanonaphthalen-9-one, 1,4,4a,5,6,7,8,8a-octahydro-, (1alpha,4alpha,4aalpha,5beta,8beta,8aalpha)-

Inchi: InChI=1S/C12H14O/c13-12-8-3-4-9(12)11-7-2-1-6(5-7)10(8)11/h1-2,6-11H,3-5H2

InchiKey: IHNUWDSCTBUWKK-UHFFFAOYSA-N

Formula: C12H14O

SMILES: O=C1C2CCC1C1C3C=CC(C3)C21

Mol. weight [g/mol]: 174.24

CAS: 36204-31-6

Physical Properties

Property code	Value	Unit	Source
gf	185.11	kJ/mol	Joback Method
hf	-120.41	kJ/mol	Joback Method
hfus	22.25	kJ/mol	Joback Method
hvap	45.88	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.78	eV	NIST Webbook
log10ws	-2.11		Crippen Method
logp	2.034		Crippen Method
mcvol	133.770	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	558.56	K	Joback Method
tc	792.38	K	Joback Method
tf	357.26	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.22	J/mol×K	558.56	Joback Method
cpg	395.26	J/mol×K	597.53	Joback Method
cpg	413.80	J/mol×K	636.50	Joback Method
cpg	430.99	J/mol×K	675.47	Joback Method
cpg	446.94	J/mol×K	714.44	Joback Method
cpg	461.79	J/mol×K	753.41	Joback Method

cpg	475.67	J/mol×K	792.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36204316&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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume