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

Other names: 1,4:5,8-Dimethanonaphthalen-9-one, (1«alpha»,4«alpha»,4a«alpha»,5«beta»,8«beta»,8a«alpha»)-

Inchi: InChI=1S/C12H16O/c13-12-8-3-4-9(12)11-7-2-1-6(5-7)10(8)11/h6-11H,1-5H2

InchiKey: BXCXSNWNIVXFED-UHFFFAOYSA-N

Formula: C12H16O

SMILES: O=C1C2CCC1C1C3CCC(C3)C21

Mol. weight [g/mol]: 176.25

CAS: 36197-31-6

Physical Properties

Property code	Value	Unit	Source
gf	155.15	kJ/mol	Joback Method
hf	-178.19	kJ/mol	Joback Method
hfus	21.03	kJ/mol	Joback Method
hvap	45.59	kJ/mol	Joback Method
ie	8.78	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-2.25		Crippen Method
logp	2.258		Crippen Method
mcvol	138.070	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	559.40	K	Joback Method
tc	790.88	K	Joback Method
tf	356.50	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.50	J/mol×K	559.40	Joback Method
cpg	415.74	J/mol×K	597.98	Joback Method
cpg	435.46	J/mol×K	636.56	Joback Method
cpg	453.79	J/mol×K	675.14	Joback Method
cpg	470.84	J/mol×K	713.72	Joback Method
cpg	486.75	J/mol×K	752.30	Joback Method

cpg	501.63	J/mol×K	790.88	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=C36197316&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
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