3,4,4a,5,8,8a-hexahydro-4a-methyl-2(1H)-naphthal

Inchi: InChI=1S/C11H16O/c1-11-6-3-2-4-9(11)8-10(12)5-7-11/h2-3,9H,4-8H2,1H3
InchiKey: OMGBHCMLAUUNBP-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CC12CC=CCC1CC(=O)CC2
Mol. weight [g/mol]: 164.24
CAS: 91967-81-6

Physical Properties

Property code	Value	Unit	Source
gf	16.72	kJ/mol	Joback Method
hf	-214.09	kJ/mol	Joback Method
hfus	6.55	kJ/mol	Joback Method
hvap	43.98	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.712		Crippen Method
mcvol	141.400	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
ripol	1952.00		NIST Webbook
tb	548.86	K	Joback Method
tc	796.36	K	Joback Method
tf	328.41	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.64	J/mol×K	548.86	Joback Method
cpg	375.20	J/mol×K	590.11	Joback Method
cpg	394.34	J/mol×K	631.36	Joback Method
cpg	412.22	J/mol×K	672.61	Joback Method
cpg	429.00	J/mol×K	713.86	Joback Method
cpg	444.85	J/mol×K	755.11	Joback Method
cpg	459.92	J/mol×K	796.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91967816&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume