cis-octahydronaphthalene-2(1H)-one

Other names: 2(1H)-Naphthalenone, octahydro-, cis-
Inchi: InChI=1S/C10H16O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h8-9H,1-7H2/t8-,9+/m0/s1
InchiKey: LGVJRKCQQHOWAU-DTWKUNHWSA-N
Formula: C10H16O
SMILES: O=C1CCC2CCCCC2C1
Mol. weight [g/mol]: 152.23
CAS: 1579-21-1

Physical Properties

Property code	Value	Unit	Source
chl	-5862.70 ± 4.50	kJ/mol	NIST Webbook
chl	-5867.20	kJ/mol	NIST Webbook
gf	-16.17	kJ/mol	Joback Method
hf	-266.47	kJ/mol	Joback Method
hfus	9.04	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.546		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	526.58	K	Joback Method
tc	766.02	K	Joback Method
tf	292.48	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.13	J/mol×K	526.58	Joback Method
cpg	346.46	J/mol×K	566.49	Joback Method
cpg	366.51	J/mol×K	606.39	Joback Method
cpg	385.29	J/mol×K	646.30	Joback Method
cpg	402.83	J/mol×K	686.21	Joback Method
cpg	419.17	J/mol×K	726.11	Joback Method

cpg	434.33	J/mol×K	766.02	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=C1579211&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume