

Cyclopropa[d]naphthalen-2(4aH)-one, 1,1a,5,6,7,8-hexahydro-4a,8,8-trimethyl-, [1aR-(1a«alpha»,4a«beta»,8aS)-]

Other names: Cyclopropa[d]naphthalen-2(4aH)-one, 1,1a,5,6,7,8-hexahydro-4a,8,8-trimethyl-,
Mayuron

Inchi:	InChI=1S/C14H20O/c1-12(2)6-4-7-13(3)8-5-11(15)10-9-14(10,12)13/h5,8,10H,4,6-7,9H2
InchiKey:	MPIBOQKDJNGGSK-UHFFFAOYSA-N
Formula:	C14H20O
SMILES:	CC1(C)CCCC2(C)C=CC(=O)C3CC312
Mol. weight [g/mol]:	204.31
CAS:	4677-90-1

Physical Properties

Property code	Value	Unit	Source
gf	108.24	kJ/mol	Joback Method
hf	-180.75	kJ/mol	Joback Method
hfus	5.13	kJ/mol	Joback Method
hvap	47.62	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.348		Crippen Method
mcvol	172.810	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
ripol	1992.00		NIST Webbook
ripol	1992.00		NIST Webbook
tb	611.51	K	Joback Method
tc	864.31	K	Joback Method
tf	430.76	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.35	J/molxK	611.51	Joback Method
cpg	507.23	J/molxK	653.64	Joback Method
cpg	526.92	J/molxK	695.78	Joback Method
cpg	545.93	J/molxK	737.91	Joback Method

cpg	564.79	J/mol×K	780.05	Joback Method
cpg	584.01	J/mol×K	822.18	Joback Method
cpg	604.10	J/mol×K	864.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4677901&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

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