Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-, (4«alpha»,4a«alpha»,7«alpha»,7a«alpha»)-

Other names: Cyclopenta[c]pyran-1(3H)-one, hexahydro-4«alpha»,7«alpha»-dimethyl-, «alpha»-Dihydronepetalactone
Isodihydronepetalactone
Isonepetalactone, dihydro-
Nepetalactone, «alpha»-dihydro-
Nepetalactone, isodihydro-
4«alpha»,7«alpha»-Dimethylhexahydrocyclopenta[c]pyran-1(3H)-one
3,4«alpha»-dihydro-4a«alpha»,7«alpha»,7a«alpha»-Nepetalactone
Dihydronepetalactone

Inchi: InChI=1S/C10H16O2/c1-6-3-4-8-7(2)5-12-10(11)9(6)8/h6-9H,3-5H2,1-2H3/t6-,7-,8+,9+/m

InchiKey: LSRNBGXEEKNZHN-HXFLIBJXSA-N

Formula: C10H16O2

SMILES: CC1COC(=O)C2C(C)CCC12

Mol. weight [g/mol]: 168.23

CAS: 17672-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-105.61	kJ/mol	Joback Method
hf	-432.99	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	46.34	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.842		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	1397.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1414.00		NIST Webbook
ripol	1992.00		NIST Webbook
ripol	1992.00		NIST Webbook
tb	539.92	K	Joback Method
tc	767.98	K	Joback Method

tf	314.09	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.98	J/mol×K	539.92	Joback Method
cpg	379.23	J/mol×K	577.93	Joback Method
cpg	398.36	J/mol×K	615.94	Joback Method
cpg	416.39	J/mol×K	653.95	Joback Method
cpg	433.33	J/mol×K	691.96	Joback Method
cpg	449.20	J/mol×K	729.97	Joback Method
cpg	464.00	J/mol×K	767.98	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=C17672967&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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