

4a«alpha»,7«alpha»,7a«alpha»-Nepetalactone

Other names:	cis,cis-Nepetalactone Nepetalactone, 4aa,7a,7aa
Inchi:	InChI=1S/C10H14O2/c1-6-3-4-8-7(2)5-12-10(11)9(6)8/h5-6,8-9H,3-4H2,1-2H3/t6-,8+,9+
InchiKey:	ZDKZHVNKFOXMND-YEPSODPASA-N
Formula:	C10H14O2
SMILES:	CC1=COC(=O)C2C(C)CCC12
Mol. weight [g/mol]:	166.22

Physical Properties

Property code	Value	Unit	Source
gf	-77.57	kJ/mol	Joback Method
hf	-366.34	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	47.60	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.109		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1371.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1322.00		NIST Webbook
tb	548.73	K	Joback Method
tc	780.29	K	Joback Method
tf	331.61	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.65	J/mol×K	548.73	Joback Method
cpg	357.85	J/mol×K	587.32	Joback Method
cpg	375.01	J/mol×K	625.92	Joback Method
cpg	391.16	J/mol×K	664.51	Joback Method
cpg	406.31	J/mol×K	703.10	Joback Method
cpg	420.46	J/mol×K	741.70	Joback Method
cpg	433.65	J/mol×K	780.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

vc: Critical Volume

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