

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

Other names:	Nepetalactone, 4aa,7a,7ab
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-/r
InchiKey:	ZDKZHVNKFOXMND-BWVDBABLSA-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	1390.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1357.00		NIST Webbook
tb	548.73	K	Joback Method
tc	780.29	K	Joback Method
tf	331.61	K	Joback Method
vc	0.498	m ³ /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

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=R285722&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/13-902-5/4a-alpha-7-alpha-7a-beta-Nepetalactone.pdf>

Generated by Cheméo on 2024-04-25 20:10:21.673141716 +0000 UTC m=+16365070.593719028.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.