2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3«alpha»,5a«alpha»,9«alpha»,9a«alpha»)]-

Other names:	(3R,5aS,9R,9aS)-2,2,5a,9-Tetramethyloctahydro-2H-3,9a-methanobenzo[b]oxepine
	Dihydro-«beta»-agarofuran
	«beta»-Agarofuran, dihydro-
	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-
	«beta»-Dihydroagarofuran
	Dihydroagarofuran
	trans-Dihydroagarofuran
	Deoxybaimuxino
	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, (3R,5aS,9R,9aS)-
	«beta»-Dihydroagarofurane
	Dihydro-«beta»-agarofurane
Inchi:	InChI=1S/C15H26O/c1-11-6-5-8-14(4)9-7-12-10-15(11,14)16-13(12,2)3/h11-12H,5-10H2
InchiKey:	HVAVUZLEYSAYGE-XQKBIRTKSA-N
Formula:	C15H26O
SMILES:	CC1CCCC2(C)CCC3CC12OC3(C)C
Mol. weight [g/mol]:	222.37
CAS:	5956-09-2

Physical Properties

Property code	Value	Unit	Source
gf	103.36	kJ/mol	Joback Method
hf	-279.97	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	49.68	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.160		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1479.00		NIST Webbook

rinpol	1496.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1706.00		NIST Webbook
tb	593.96	K	Joback Method
tc	830.88	K	Joback Method
tf	391.86	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.99	J/mol×K	593.96	Joback Method
cpg	583.21	J/mol×K	633.45	Joback Method
cpg	605.88	J/mol×K	672.93	Joback Method
cpg	627.44	J/mol×K	712.42	Joback Method
cpg	648.34	J/mol×K	751.91	Joback Method
cpg	669.02	J/mol×K	791.40	Joback Method
cpg	689.92	J/mol×K	830.88	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=C5956092&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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