

«gamma»-(E)-Atlantone

Other names:	(E)-«gamma»-Atlantone
Inchi:	InChI=1S/C15H22O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5,9H,6-8,10H2,1-4H3
InchiKey:	QEAHSEZXAQIWSW-YPKPFQOOSA-N
Formula:	C15H22O
SMILES:	CC(C)=CC(=O)CC(C)=C1CC=C(C)CC1
Mol. weight [g/mol]:	218.33
CAS:	108549-47-9

Physical Properties

Property code	Value	Unit	Source
gf	107.57	kJ/mol	Joback Method
hf	-170.87	kJ/mol	Joback Method
hfus	25.71	kJ/mol	Joback Method
hvap	58.33	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.359		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1711.50		NIST Webbook
tb	635.39	K	Joback Method
tc	851.73	K	Joback Method
tf	311.00	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.34	J/molxK	635.39	Joback Method
cpg	537.66	J/molxK	671.45	Joback Method
cpg	554.87	J/molxK	707.50	Joback Method
cpg	571.03	J/molxK	743.56	Joback Method

cpg	586.20	J/mol×K	779.62	Joback Method
cpg	600.44	J/mol×K	815.68	Joback Method
cpg	613.82	J/mol×K	851.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108549479&Units=SI
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

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
hvp:	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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