2,6,10-Cycloundecatrien-1-one, 2,6,9,9-tetramethyl-, (E,E,E)-

Other names: Zerumbone
Zerumbene

Inchi: InChI=1S/C15H22O/c1-12-6-5-7-13(2)14(16)9-11-15(3,4)10-8-12/h7-9,11H,5-6,10H2,1-4

InchiKey: GIHNTRQPEMKFKO-RTTFEGKLSA-N

Formula: C15H22O

SMILES: CC1=CCC(C)(C)C=CC(=O)C(C)=CCC1

Mol. weight [g/mol]: 218.33

CAS: 471-05-6

Physical Properties

Property code	Value	Unit	Source
gf	-18.09	kJ/mol	Joback Method
hf	-301.47	kJ/mol	Joback Method
hfus	12.04	kJ/mol	Joback Method
hvap	55.57	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1753.93		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1732.00		NIST Webbook
ripol	2273.00		NIST Webbook
tb	659.00	K	Joback Method
tc	908.29	K	Joback Method
tf	368.03	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.35	J/mol×K	659.00	Joback Method
cpg	563.31	J/mol×K	700.55	Joback Method
cpg	584.92	J/mol×K	742.10	Joback Method
cpg	605.27	J/mol×K	783.64	Joback Method
cpg	624.42	J/mol×K	825.19	Joback Method
cpg	642.46	J/mol×K	866.74	Joback Method
cpg	659.45	J/mol×K	908.29	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C471056&Units=SI
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

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