2,6,9,11-Dodecatetraenal, 2,6,10-trimethyl-, (E,E,E)-

Other names: «alpha»-Sinensal
(E,E,E)-2,6,10-trimethyldodeca-2,6,9,11-tetraen-1-al
Inchi: InChI=1S/C15H22O/c1-5-13(2)8-6-9-14(3)10-7-11-15(4)12-16/h5,8-9,11-12H,1,6-7,10H2
InchiKey: PFSTYGCNVAVZBK-JQGMZEBDSA-N
Formula: C15H22O
SMILES: C=CC(C)=CCC=C(C)CCC=C(C)C=O
Mol. weight [g/mol]: 218.33
CAS: 17909-77-2

Physical Properties

Property code	Value	Unit	Source
gf	278.75	kJ/mol	Joback Method
hf	9.21	kJ/mol	Joback Method
hfus	32.29	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.381		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	1748.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1759.60		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1748.00		NIST Webbook

rinpol	1726.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1750.00		NIST Webbook
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rinpol	1753.00		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1759.60		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1765.00		NIST Webbook
ripol	2304.00		NIST Webbook
ripol	2268.00		NIST Webbook
ripol	2323.00		NIST Webbook
ripol	2268.00		NIST Webbook
ripol	2313.00		NIST Webbook
ripol	2268.00		NIST Webbook
ripol	2323.00		NIST Webbook
ripol	2340.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2304.00		NIST Webbook
ripol	2304.00		NIST Webbook
ripol	2323.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2323.00		NIST Webbook
ripol	2323.00		NIST Webbook
ripol	2268.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2261.00		NIST Webbook
tb	600.06	K	Joback Method
tc	794.25	K	Joback Method
tf	241.93	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.33	J/mol×K	600.06	Joback Method
cpg	525.67	J/mol×K	632.43	Joback Method
cpg	541.10	J/mol×K	664.79	Joback Method
cpg	555.67	J/mol×K	697.16	Joback Method
cpg	569.45	J/mol×K	729.52	Joback Method
cpg	582.51	J/mol×K	761.89	Joback Method
cpg	594.92	J/mol×K	794.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17909772&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
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
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

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