2,6,10-Dodecatrienal, 3,7,11-trimethyl-, (E,E)-

Other names:	(E,E)-3,7,11-Trimethyl-2,6,10-dodecatrienal trans,trans-Farnesal trans,trans-2,6-Farnesal E,E-Farnesal Farnesal, trans,trans- 2,6-trans-trans-Farnesal (2E,6E)-Farnesal (2E,6E)-3,7,11-Trimethyl-2,6,10-dodecatrienal 3,7,11-trimethyl-2,6,10-Dodecatrienal, (trans,trans)- Farnesal, (E,E)- trans-Farnesal 2,6,10-Dodecatrienal, 3,7,11-trimethyl-, (2E,6E)- farnesyl aldehyde 3,7,11-trimethyl-2,6,10-dodecatrienal (farnesal) Farnesal
Inchi:	InChI=1S/C15H24O/c1-13(2)7-5-8-14(3)9-6-10-15(4)11-12-16/h7,9,11-12H,5-6,8,10H2,1
InchiKey:	YHRUHBBTQZKMEX-YFVJMOTDSA-N
Formula:	C15H24O
SMILES:	CC(C)=CCCC(C)=CCCC(C)=CC=O
Mol. weight [g/mol]:	220.35
CAS:	502-67-0

Physical Properties

Property code	Value	Unit	Source
gf	190.91	kJ/mol	Joback Method
hf	-116.22	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	55.82	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.605		Crippen Method
mcvol	210.880	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	1737.50		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1738.00		NIST Webbook
rinpol	1733.00		NIST Webbook

rinpol	1715.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1737.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1735.00		NIST Webbook
ripol	2314.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2268.00		NIST Webbook
tb	603.38	K	Joback Method
tc	794.15	K	Joback Method
tf	243.69	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.64	J/mol×K	603.38	Joback Method
cpg	547.51	J/mol×K	635.18	Joback Method
cpg	563.47	J/mol×K	666.97	Joback Method
cpg	578.59	J/mol×K	698.77	Joback Method
cpg	592.93	J/mol×K	730.56	Joback Method
cpg	606.55	J/mol×K	762.36	Joback Method
cpg	619.50	J/mol×K	794.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.50 ± 1.50	K	0.05	NIST Webbook

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=C502670&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume