2,6,9,11-Dodecatetraenal, 2,6,10-trimethyl-

Other names: 2,6,10-Trimethyl-2,6,9,11-dodecatetraenal
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-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=CC(C)=CCC=C(C)CCC=C(C)C=O
Mol. weight [g/mol]: 218.33
CAS: 4955-32-2

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	1686.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1719.00		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=C4955322&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume