(E,E,E)-2,4,6-dodecatrienal

Inchi: InChI=1S/C12H18O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h6-12H,2-5H2,1H3/b7-6+,9-8+,11-1
InchiKey: IZNAXSQBWJPYHG-OBWVEWQSSA-N
Formula: C12H18O
SMILES: CCCCCC=CC=CC=O
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	191.30	kJ/mol	Joback Method
hf	-24.93	kJ/mol	Joback Method
hfus	29.73	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.434		Crippen Method
mcvol	168.610	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
ripol	2216.00		NIST Webbook
ripol	2216.00		NIST Webbook
tb	535.10	K	Joback Method
tc	723.30	K	Joback Method
tf	251.76	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.90	J/mol×K	535.10	Joback Method
cpg	448.00	J/mol×K	691.94	Joback Method
cpg	436.40	J/mol×K	660.57	Joback Method
cpg	424.14	J/mol×K	629.20	Joback Method
cpg	411.17	J/mol×K	597.83	Joback Method
cpg	397.44	J/mol×K	566.47	Joback Method

cpg	459.00	J/mol×K	723.30	Joback Method
dvisc	0.0001538	Pa×s	535.10	Joback Method
dvisc	0.0002039	Pa×s	487.88	Joback Method
dvisc	0.0002874	Pa×s	440.65	Joback Method
dvisc	0.0004398	Pa×s	393.43	Joback Method
dvisc	0.0007558	Pa×s	346.21	Joback Method
dvisc	0.0015411	Pa×s	298.98	Joback Method
dvisc	0.0041052	Pa×s	251.76	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R236963&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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