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

Inchi: InChI=1S/C11H16O/c1-2-3-4-5-6-7-8-9-10-11-12/h5-11H,2-4H2,1H3/b6-5+,8-7+,10-9+
InchiKey: IYJQORLVRUQEIH-SUTYWZMXSA-N
Formula: C11H16O
SMILES: CCCCC=CC=CC=CC=O
Mol. weight [g/mol]: 164.24

Physical Properties

Property code	Value	Unit	Source
gf	182.88	kJ/mol	Joback Method
hf	-4.29	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Joback Method
hvap	46.67	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.044		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1498.00		NIST Webbook
ripol	2106.00		NIST Webbook
ripol	2106.00		NIST Webbook
tb	512.22	K	Joback Method
tc	702.68	K	Joback Method
tf	240.49	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.68	J/mol×K	512.22	Joback Method
cpg	398.37	J/mol×K	670.94	Joback Method
cpg	387.42	J/mol×K	639.19	Joback Method
cpg	375.83	J/mol×K	607.45	Joback Method
cpg	363.54	J/mol×K	575.71	Joback Method
cpg	350.51	J/mol×K	543.96	Joback Method
cpg	408.72	J/mol×K	702.68	Joback Method

dvisc	0.0001639	Pa×s	512.22	Joback Method
dvisc	0.0002163	Pa×s	466.93	Joback Method
dvisc	0.0003032	Pa×s	421.64	Joback Method
dvisc	0.0004609	Pa×s	376.36	Joback Method
dvisc	0.0007858	Pa×s	331.07	Joback Method
dvisc	0.0015863	Pa×s	285.78	Joback Method
dvisc	0.0041723	Pa×s	240.49	Joback Method

Sources

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=R236998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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