(E,E)-2,4-Octadienal

Inchi: InChI=1S/C8H12O/c1-2-3-4-5-6-7-8-9/h4-8H,2-3H2,1H3/b5-4+,7-6+
InchiKey: DVVATNQISMINCX-YTXTXJHMSA-N
Formula: C8H12O
SMILES: CCCC=CC=CC=O
Mol. weight [g/mol]: 124.18

Physical Properties

Property code	Value	Unit	Source
gf	77.40	kJ/mol	Joback Method
hf	-59.59	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	40.04	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1111.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1108.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1616.00		NIST Webbook
tb	439.42	K	Joback Method
tc	627.33	K	Joback Method
tf	211.76	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.21	J/mol×K	439.42	Joback Method
cpg	236.72	J/mol×K	470.74	Joback Method

cpg	247.60	J/mol×K	502.06	Joback Method
cpg	257.87	J/mol×K	533.38	Joback Method
cpg	267.58	J/mol×K	564.70	Joback Method
cpg	276.76	J/mol×K	596.01	Joback Method
cpg	285.43	J/mol×K	627.33	Joback Method
dvisc	0.0042123	Pa×s	211.76	Joback Method
dvisc	0.0017693	Pa×s	249.70	Joback Method
dvisc	0.0009343	Pa×s	287.65	Joback Method
dvisc	0.0005725	Pa×s	325.59	Joback Method
dvisc	0.0003886	Pa×s	363.53	Joback Method
dvisc	0.0002838	Pa×s	401.48	Joback Method
dvisc	0.0002188	Pa×s	439.42	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=R604970&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