2,4-octadienal

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

Physical Properties

Property code	Value	Unit	Source
af	0.3606		Cheméo Relay (1.0)
gf	77.40	kJ/mol	Joback Method
hf	-124.39	kJ/mol	Cheméo Relay (1.0)
hfus	19.17	kJ/mol	Joback Method
hvap	51.27	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
log10ws	-1.99		Cheméo Relay (1.0)
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1125.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1082.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1569.00		NIST Webbook
tb	443.84	K	Cheméo Relay (1.0)

tc	637.66	K	Cheméo Relay (1.0)
tf	266.16	K	Cheméo Relay (1.0)
vc	0.417	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.21	J/mol×K	439.42	Joback Method
cpg	285.43	J/mol×K	627.33	Joback Method
cpg	276.76	J/mol×K	596.01	Joback Method
cpg	267.58	J/mol×K	564.70	Joback Method
cpg	257.87	J/mol×K	533.38	Joback Method
cpg	247.60	J/mol×K	502.06	Joback Method
cpg	236.72	J/mol×K	470.74	Joback Method
dvisc	0.0005725	Pa×s	325.59	Joback Method
dvisc	0.0002188	Pa×s	439.42	Joback Method
dvisc	0.0002838	Pa×s	401.48	Joback Method
dvisc	0.0003886	Pa×s	363.53	Joback Method
dvisc	0.0042123	Pa×s	211.76	Joback Method
dvisc	0.0009343	Pa×s	287.65	Joback Method
dvisc	0.0017693	Pa×s	249.70	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R75517&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

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
ie:	Ionization energy
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