2,5-Octadienal, (Z,Z)

Inchi: InChI=1S/C8H12O/c1-2-3-4-5-6-7-8-9/h3-4,6-8H,2,5H2,1H3/b4-3-,7-6-
InchiKey: YUPOVSHIQPPPSA-CWWKMNTPSA-N
Formula: C8H12O
SMILES: CCC=CCC=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
ripol	1425.00		NIST Webbook
ripol	1425.00		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=R211528&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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