

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:	YUPOVSHIQPPSA-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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.21	J/molxK	439.42	Joback Method
cpg	236.72	J/molxK	470.74	Joback Method
cpg	247.60	J/molxK	502.06	Joback Method
cpg	257.87	J/molxK	533.38	Joback Method
cpg	267.58	J/molxK	564.70	Joback Method
cpg	276.76	J/molxK	596.01	Joback Method
cpg	285.43	J/molxK	627.33	Joback Method
dvisc	0.0042123	Paxs	211.76	Joback Method

dvisc	0.0017693	Paxs	249.70	Joback Method
dvisc	0.0009343	Paxs	287.65	Joback Method
dvisc	0.0005725	Paxs	325.59	Joback Method
dvisc	0.0003886	Paxs	363.53	Joback Method
dvisc	0.0002838	Paxs	401.48	Joback Method
dvisc	0.0002188	Paxs	439.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R211528&Units=SI

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rip_{ol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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