

(E,Z)-2,4-Heptadienal

Inchi:	InChI=1S/C7H10O/c1-2-3-4-5-6-7-8/h3-7H,2H2,1H3/b4-3+,6-5+
InchiKey:	SATICYYAWWYRAM-VNKDHWASSA-N
Formula:	C7H10O
SMILES:	CCC=CC=CC=O
Mol. weight [g/mol]:	110.15

Physical Properties

Property code	Value	Unit	Source
gf	68.98	kJ/mol	Joback Method
hf	-38.95	kJ/mol	Joback Method
hfus	16.58	kJ/mol	Joback Method
hvap	37.81	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.708		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	968.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	999.00		NIST Webbook
tb	416.54	K	Joback Method
tc	606.14	K	Joback Method
tf	200.49	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.30	J/molxK	416.54	Joback Method
cpg	232.55	J/molxK	574.54	Joback Method
cpg	224.36	J/molxK	542.94	Joback Method
cpg	215.67	J/molxK	511.34	Joback Method
cpg	206.45	J/molxK	479.74	Joback Method

cpg	196.67	J/mol×K	448.14	Joback Method
cpg	240.28	J/mol×K	606.14	Joback Method
dvisc	0.0002197	Paxs	416.54	Joback Method
dvisc	0.0002831	Paxs	380.53	Joback Method
dvisc	0.0003844	Paxs	344.52	Joback Method
dvisc	0.0005608	Paxs	308.51	Joback Method
dvisc	0.0009040	Paxs	272.51	Joback Method
dvisc	0.0016852	Paxs	236.50	Joback Method
dvisc	0.0039290	Paxs	200.49	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=R604950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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