(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	999.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	968.00		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/mol×K	416.54	Joback Method
cpg	196.67	J/mol×K	448.14	Joback Method
cpg	206.45	J/mol×K	479.74	Joback Method
cpg	215.67	J/mol×K	511.34	Joback Method
cpg	224.36	J/mol×K	542.94	Joback Method

cpg	232.55	J/mol×K	574.54	Joback Method
cpg	240.28	J/mol×K	606.14	Joback Method
dvisc	0.0039290	Pa×s	200.49	Joback Method
dvisc	0.0016852	Pa×s	236.50	Joback Method
dvisc	0.0009040	Pa×s	272.51	Joback Method
dvisc	0.0005608	Pa×s	308.51	Joback Method
dvisc	0.0003844	Pa×s	344.52	Joback Method
dvisc	0.0002831	Pa×s	380.53	Joback Method
dvisc	0.0002197	Pa×s	416.54	Joback Method

Sources

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

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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