(E,Z)-2,4-heptadienal

Other names: 2,4-Heptadienal, (E,Z)-
(E; Z)-2,4-heptadienal
(E)-2,(Z)-4-heptadienal
(E,Z)-Hepta-2,4-dienal
trans-2,cis-4-heptadienal
Inchi: InChI=1S/C7H10O/c1-2-3-4-5-6-7-8/h3-7H,2H2,1H3/b4-3-,6-5+
InchiKey: SATICYYAWWYRAM-DNVGVPOPSA-N
Formula: C7H10O
SMILES: CCC=CC=CC=O
Mol. weight [g/mol]: 110.15
CAS: 4313-02-4

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	971.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	1004.00		NIST Webbook

rinpol	1011.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	985.00	NIST Webbook
rinpol	996.00	NIST Webbook
rinpol	980.00	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	973.00	NIST Webbook
rinpol	979.00	NIST Webbook
rinpol	1013.00	NIST Webbook
ripol	1479.00	NIST Webbook
ripol	1479.00	NIST Webbook
ripol	1479.00	NIST Webbook
ripol	1479.00	NIST Webbook
ripol	1430.00	NIST Webbook
ripol	1435.00	NIST Webbook
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ripol	1436.00	NIST Webbook
ripol	1453.00	NIST Webbook
ripol	1455.00	NIST Webbook
ripol	1460.00	NIST Webbook
ripol	1458.00	NIST Webbook
ripol	1457.00	NIST Webbook
ripol	1471.00	NIST Webbook
ripol	1479.00	NIST Webbook
ripol	1460.00	NIST Webbook
ripol	1479.00	NIST Webbook
ripol	1479.00	NIST Webbook
ripol	1459.00	NIST Webbook
ripol	1454.00	NIST Webbook
ripol	1430.00	NIST Webbook
ripol	1430.00	NIST Webbook
ripol	1480.00	NIST Webbook
ripol	1450.00	NIST Webbook
ripol	1469.00	NIST Webbook
ripol	1478.00	NIST Webbook
ripol	1479.00	NIST Webbook
ripol	1479.00	NIST Webbook

ripol	1479.00		NIST Webbook
ripol	1479.00		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

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=C4313024&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
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

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