3,5-Heptadienal, 2-ethylidene-6-methyl-

Other names:	(2E,3Z)-2-Ethylidene-6-methyl-3,5-heptadienal
Inchi:	InChI=1S/C10H14O/c1-4-10(8-11)7-5-6-9(2)3/h4-8H,1-3H3/b7-5-,10-4+
InchiKey:	GNLLTRIMWRZWBF-ACUVPTBSSA-N
Formula:	C10H14O
SMILES:	CC=C(C=O)C=CC=C(C)C
Mol. weight [g/mol]:	150.22
CAS:	99172-18-6

Physical Properties

Property code	Value	Unit	Source
gf	157.36	kJ/mol	Joback Method
hf	-3.23	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.654		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1395.00		NIST Webbook
tb	489.10	K	Joback Method
tc	689.18	K	Joback Method
tf	201.30	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.00	J/mol×K	489.10	Joback Method
cpg	305.44	J/mol×K	522.45	Joback Method
cpg	318.05	J/mol×K	555.79	Joback Method
cpg	329.88	J/mol×K	589.14	Joback Method
cpg	340.99	J/mol×K	622.49	Joback Method
cpg	351.44	J/mol×K	655.84	Joback Method
cpg	361.27	J/mol×K	689.18	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=C99172186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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