2,4-Heptadienal, 2,4-dimethyl-

Other names:	2,4-Dimethyl-2,4-heptadienal
Inchi:	InChI=1S/C9H14O/c1-4-5-8(2)6-9(3)7-10/h5-7H,4H2,1-3H3/b8-5+,9-6+
InchiKey:	PHOBFHQBEYNKAL-XVYDYJIPSA-N
Formula:	C9H14O
SMILES:	CCC=C(C)C=C(C)C=O
Mol. weight [g/mol]:	138.21
CAS:	42452-48-2

Physical Properties

Property code	Value	Unit	Source
gf	68.72	kJ/mol	Joback Method
hf	-99.81	kJ/mol	Joback Method
hfus	19.14	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.488		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1090.00		NIST Webbook
tb	462.06	K	Joback Method
tc	655.30	K	Joback Method
tf	195.11	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.06	J/mol×K	462.06	Joback Method
cpg	278.99	J/mol×K	494.27	Joback Method
cpg	291.21	J/mol×K	526.47	Joback Method
cpg	302.74	J/mol×K	558.68	Joback Method
cpg	313.64	J/mol×K	590.88	Joback Method

cpg	323.93	J/mol×K	623.09	Joback Method
cpg	333.66	J/mol×K	655.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42452482&Units=SI
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

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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