5-Heptenal, 2,6-dimethyl-

Other names:	2,6-Dimethyl hept-5-en-1-al
	2,6-Dimethyl-5-hepten-1-al
	2,6-Dimethyl-5-heptenal
	2,6-Dimethylhept-5-enal
	Bergamal
	Melonal
Inchi:	InChI=1S/C9H16O/c1-8(2)5-4-6-9(3)7-10/h5,7,9H,4,6H2,1-3H3
InchiKey:	YGFGZTXGYTUXBA-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	CC(C)=CCCC(C)C=O
Mol. weight [g/mol]:	140.22
CAS:	106-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-5.39	kJ/mol	Joback Method
hf	-212.52	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Joback Method
hvap	42.00	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.568		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1044.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1039.00		NIST Webbook

rinpol	1060.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1037.70		NIST Webbook
rinpol	1038.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1389.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1315.00		NIST Webbook
tb	457.58	K	Joback Method
tc	642.53	K	Joback Method
tf	199.15	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.58	J/mol×K	457.58	Joback Method
cpg	296.03	J/mol×K	488.40	Joback Method
cpg	308.83	J/mol×K	519.23	Joback Method
cpg	321.02	J/mol×K	550.05	Joback Method
cpg	332.61	J/mol×K	580.88	Joback Method
cpg	343.63	J/mol×K	611.70	Joback Method
cpg	354.11	J/mol×K	642.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	13.30	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32166e+01
Coeff. B	-3.54204e+03
Coeff. C	-6.79600e+01
Temperature range (K), min.	341.92
Temperature range (K), max.	516.03

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C106729&Units=SI

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume