Hexanal, 3,5,5-trimethyl-

Other names:	3,5,5-Trimethyl n-hexanal
	3,5,5-Trimethylhexanal
	Isonylaldehyde
	tert-Butylisopentanal
Inchi:	InChI=1S/C9H18O/c1-8(5-6-10)7-9(2,3)4/h6,8H,5,7H2,1-4H3
InchiKey:	WTPYRCJDOZVZON-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	CC(CC=O)CC(C)(C)C
Mol. weight [g/mol]:	142.24
CAS:	5435-64-3

Physical Properties

Property code	Value	Unit	Source
gf	-74.22	kJ/mol	Joback Method
hf	-328.70	kJ/mol	Joback Method
hfus	10.42	kJ/mol	Joback Method
hvap	40.66	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.648		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	963.00		NIST Webbook
rinpol	963.00		NIST Webbook
ripol	1200.00		NIST Webbook
tb	450.31	K	Joback Method
tc	634.52	K	Joback Method
tf	220.61	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.10	J/mol×K	450.31	Joback Method
cpg	367.97	J/mol×K	603.82	Joback Method

cpg	355.98	J/mol×K	573.12	Joback Method
cpg	343.32	J/mol×K	542.42	Joback Method
cpg	329.97	J/mol×K	511.71	Joback Method
cpg	315.91	J/mol×K	481.01	Joback Method
cpg	379.34	J/mol×K	634.52	Joback Method
dvisc	0.0002975	Pa×s	450.31	Joback Method
dvisc	0.0004163	Pa×s	412.03	Joback Method
dvisc	0.0006241	Pa×s	373.74	Joback Method
dvisc	0.0010263	Pa×s	335.46	Joback Method
dvisc	0.0019183	Pa×s	297.18	Joback Method
dvisc	0.0043144	Pa×s	258.89	Joback Method
dvisc	0.0128554	Pa×s	220.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.70	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50694e+01
Coeff. B	-4.12718e+03
Coeff. C	-6.80910e+01
Temperature range (K), min.	347.30
Temperature range (K), max.	491.05

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=C5435643&Units=SI
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

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
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

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