

Hexanal, 3,3-dimethyl-

Other names:	3,3-Dimethyl-hexanal
Inchi:	InChI=1S/C8H16O/c1-4-5-8(2,3)6-7-9/h7H,4-6H2,1-3H3
InchiKey:	IHEORNQYISDNQZ-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CCCC(C)(C)CC=O
Mol. weight [g/mol]:	128.21
CAS:	55320-57-5

Physical Properties

Property code	Value	Unit	Source
gf	-80.20	kJ/mol	Joback Method
hf	-302.78	kJ/mol	Joback Method
hfus	11.35	kJ/mol	Joback Method
hvap	38.83	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	427.87	K	Joback Method
tc	609.54	K	Joback Method
tf	224.34	K	Joback Method
vc	0.489	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.85	J/mol×K	427.87	Joback Method
cpg	272.30	J/mol×K	458.15	Joback Method
cpg	285.08	J/mol×K	488.43	Joback Method
cpg	297.22	J/mol×K	518.71	Joback Method
cpg	308.74	J/mol×K	548.98	Joback Method
cpg	319.67	J/mol×K	579.26	Joback Method
cpg	330.03	J/mol×K	609.54	Joback Method
dvisc	0.0079397	Paxs	224.34	Joback Method

dvisc	0.0033052	Paxs	258.26	Joback Method
dvisc	0.0016864	Paxs	292.18	Joback Method
dvisc	0.0009897	Paxs	326.11	Joback Method
dvisc	0.0006422	Paxs	360.03	Joback Method
dvisc	0.0004490	Paxs	393.95	Joback Method
dvisc	0.0003322	Paxs	427.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C55320575&Units=SI

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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