

3,4-dimethylvaleraldehyde

Other names:	3,4-Dimethylpentanal
Inchi:	InChI=1S/C7H14O/c1-6(2)7(3)4-5-8/h5-7H,4H2,1-3H3
InchiKey:	SZBNDYYJXRQHA-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CC(C)C(C)CC=O
Mol. weight [g/mol]:	114.19
CAS:	19353-21-0

Physical Properties

Property code	Value	Unit	Source
gf	-96.34	kJ/mol	Joback Method
hf	-283.95	kJ/mol	Joback Method
hfus	9.13	kJ/mol	Joback Method
hvap	37.12	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.868		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	407.34	K	Joback Method
tc	587.04	K	Joback Method
tf	180.65	K	Joback Method
vc	0.432	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.96	J/mol×K	407.34	Joback Method
cpg	228.67	J/mol×K	437.29	Joback Method
cpg	239.91	J/mol×K	467.24	Joback Method
cpg	250.68	J/mol×K	497.19	Joback Method
cpg	260.99	J/mol×K	527.14	Joback Method
cpg	270.87	J/mol×K	557.09	Joback Method
cpg	280.30	J/mol×K	587.04	Joback Method
cpl	235.60	J/mol×K	323.15	NIST Webbook

dvisc	0.0134730	Paxs	180.65	Joback Method
dvisc	0.0041185	Paxs	218.43	Joback Method
dvisc	0.0017858	Paxs	256.21	Joback Method
dvisc	0.0009598	Paxs	294.00	Joback Method
dvisc	0.0005942	Paxs	331.78	Joback Method
dvisc	0.0004058	Paxs	369.56	Joback Method
dvisc	0.0002974	Paxs	407.34	Joback Method
hvapt	42.40	kJ/mol	368.00	NIST Webbook

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=C19353210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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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