3,4-Dimethylpentanal

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

Physical Properties

Property code	Value	Unit	Source
hfus	9.13	kJ/mol	Joback Method
hvap	42.26	kJ/mol	Cheméo Relay (1.0)
ie	9.72	eV	Cheméo Relay (1.0)
logp	1.868		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
tb	409.00	K	Cheméo Relay (1.0)
tf	208.65	K	Cheméo Relay (1.0)

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	0.0041185	Pa×s	218.43	Joback Method
dvisc	0.0017858	Pa×s	256.21	Joback Method
dvisc	0.0009598	Pa×s	294.00	Joback Method
dvisc	0.0005942	Pa×s	331.78	Joback Method
dvisc	0.0004058	Pa×s	369.56	Joback Method
dvisc	0.0002974	Pa×s	407.34	Joback Method

dvisc	0.0134730	Pa×s	180.65	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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19353210&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point