4-methylpentanal

Other names: Pentanal, 4-methyl-
4-methylvaleraldehyde
Inchi: InChI=1S/C6H12O/c1-6(2)4-3-5-7/h5-6H,3-4H2,1-2H3
InchiKey: JGEGJYXHCFUMJF-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CC(C)CCC=O
Mol. weight [g/mol]: 100.16
CAS: 1119-16-0

Physical Properties

Property code	Value	Unit	Source
gf	-102.32	kJ/mol	Joback Method
hf	-258.03	kJ/mol	Joback Method
hfus	10.06	kJ/mol	Joback Method
hvap	35.28	kJ/mol	Joback Method
ie	9.80	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	714.00		NIST Webbook
ripol	1038.00		NIST Webbook
ripol	1038.00		NIST Webbook
ripol	1039.00		NIST Webbook
tb	395.15 ± 2.00	K	NIST Webbook
tb	394.15 ± 3.00	K	NIST Webbook
tb	394.15 ± 2.00	K	NIST Webbook
tb	397.15 ± 3.00	K	NIST Webbook
tb	395.15 ± 1.50	K	NIST Webbook
tb	394.25 ± 1.50	K	NIST Webbook
tc	561.39	K	Joback Method
tf	184.38	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.50	J/mol×K	384.90	Joback Method
cpg	226.11	J/mol×K	531.98	Joback Method
cpg	217.54	J/mol×K	502.56	Joback Method
cpg	208.60	J/mol×K	473.15	Joback Method
cpg	199.28	J/mol×K	443.73	Joback Method
cpg	189.59	J/mol×K	414.32	Joback Method
cpg	234.32	J/mol×K	561.39	Joback Method
dvisc	0.0003084	Pa×s	384.90	Joback Method
dvisc	0.0004053	Pa×s	351.48	Joback Method
dvisc	0.0005641	Pa×s	318.06	Joback Method
dvisc	0.0008484	Pa×s	284.64	Joback Method
dvisc	0.0014226	Pa×s	251.22	Joback Method
dvisc	0.0027952	Pa×s	217.80	Joback Method
dvisc	0.0070161	Pa×s	184.38	Joback Method

Sources

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=C1119160&Units=SI

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume