(3-methyl-4-pentenal)

Inchi: InChI=1S/C6H10O/c1-3-6(2)4-5-7/h3,5-6H,1,4H2,2H3
InchiKey: MWSZRPZREJBOIP-UHFFFAOYSA-N
Formula: C6H10O
SMILES: C=CC(C)CC=O
Mol. weight [g/mol]: 98.14

Physical Properties

Property code	Value	Unit	Source
gf	-14.48	kJ/mol	Joback Method
hf	-132.60	kJ/mol	Joback Method
hfus	8.78	kJ/mol	Joback Method
hvap	34.61	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.397		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
ripol	1148.00		NIST Webbook
ripol	1148.00		NIST Webbook
tb	381.58	K	Joback Method
tc	561.84	K	Joback Method
tf	182.62	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.34	J/mol×K	381.58	Joback Method
cpg	174.78	J/mol×K	411.62	Joback Method
cpg	183.82	J/mol×K	441.67	Joback Method
cpg	192.45	J/mol×K	471.71	Joback Method
cpg	200.69	J/mol×K	501.75	Joback Method
cpg	208.56	J/mol×K	531.79	Joback Method
cpg	216.06	J/mol×K	561.84	Joback Method
dvisc	0.0058466	Pa×s	182.62	Joback Method

dvisc	0.0024354	Pa×s	215.78	Joback Method
dvisc	0.0012811	Pa×s	248.94	Joback Method
dvisc	0.0007837	Pa×s	282.10	Joback Method
dvisc	0.0005317	Pa×s	315.26	Joback Method
dvisc	0.0003883	Pa×s	348.42	Joback Method
dvisc	0.0002995	Pa×s	381.58	Joback Method

Sources

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=R218198&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume