2,2,3-Trimethyl-4-pentenal

Inchi: InChI=1S/C8H14O/c1-5-7(2)8(3,4)6-9/h5-7H,1H2,2-4H3
InchiKey: CGJMHDFLIGBWTA-UHFFFAOYSA-N
Formula: C8H14O
SMILES: C=CC(C)C(C)(C)C=O
Mol. weight [g/mol]: 126.20
CAS: 67682-09-1

Physical Properties

Property code	Value	Unit	Source
gf	5.20	kJ/mol	Joback Method
hf	-182.63	kJ/mol	Joback Method
hfus	6.55	kJ/mol	Joback Method
hvap	37.77	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	2.034		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
tb	424.11	K	Joback Method
tc	613.96	K	Joback Method
tf	207.58	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.08	J/mol×K	424.11	Joback Method
cpg	302.34	J/mol×K	582.32	Joback Method
cpg	291.84	J/mol×K	550.67	Joback Method
cpg	280.69	J/mol×K	519.03	Joback Method
cpg	268.87	J/mol×K	487.39	Joback Method
cpg	256.34	J/mol×K	455.75	Joback Method
cpg	312.24	J/mol×K	613.96	Joback Method
dvisc	0.0003172	Pa×s	424.11	Joback Method
dvisc	0.0004378	Pa×s	388.02	Joback Method

dvisc	0.0006455	Pa×s	351.93	Joback Method
dvisc	0.0010402	Pa×s	315.84	Joback Method
dvisc	0.0018957	Pa×s	279.76	Joback Method
dvisc	0.0041270	Pa×s	243.67	Joback Method
dvisc	0.0117759	Pa×s	207.58	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=C67682091&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
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