2-Pentenal, 2,4,4-trimethyl-

Other names:	2,4,4-Trimethyl-2-pentenal
Inchi:	InChI=1S/C8H14O/c1-7(6-9)5-8(2,3)4/h5-6H,1-4H3/b7-5+
InchiKey:	ANXYYWCILNEABR-FNORWQNLSA-N
Formula:	C8H14O
SMILES:	CC(C=O)=CC(C)(C)C
Mol. weight [g/mol]:	126.20
CAS:	53907-61-2

Physical Properties

Property code	Value	Unit	Source
gf	-8.53	kJ/mol	Joback Method
hf	-195.35	kJ/mol	Joback Method
hfus	10.24	kJ/mol	Joback Method
hvap	38.86	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.178		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
ripol	1254.00		NIST Webbook
ripol	1254.00		NIST Webbook
tb	431.91	K	Joback Method
tc	626.48	K	Joback Method
tf	205.30	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.32	J/mol×K	431.91	Joback Method
cpg	256.71	J/mol×K	464.34	Joback Method
cpg	269.30	J/mol×K	496.77	Joback Method
cpg	281.13	J/mol×K	529.19	Joback Method
cpg	292.25	J/mol×K	561.62	Joback Method
cpg	302.69	J/mol×K	594.05	Joback Method

cpg	312.50	J/mol×K	626.48	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=C53907612&Units=SI

Legend

cpg:	Ideal gas heat capacity
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

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