

2,2,4-Trimethyl-3-oxovaleraldehyde

Inchi:	InChI=1S/C8H14O2/c1-6(2)7(10)8(3,4)5-9/h5-6H,1-4H3
InchiKey:	MXJGWJPUNYJFQO-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC(C)C(=O)C(C)(C)C=O
Mol. weight [g/mol]:	142.20
CAS:	1482-01-5

Physical Properties

Property code	Value	Unit	Source
gf	-211.56	kJ/mol	Joback Method
hf	-420.64	kJ/mol	Joback Method
hfus	9.43	kJ/mol	Joback Method
hvap	45.18	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.437		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	481.30	K	Joback Method
tc	678.07	K	Joback Method
tf	259.27	K	Joback Method
vc	0.489	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.71	J/molxK	481.30	Joback Method
cpg	292.54	J/molxK	514.09	Joback Method
cpg	304.64	J/molxK	546.89	Joback Method
cpg	316.05	J/molxK	579.68	Joback Method
cpg	326.79	J/molxK	612.48	Joback Method
cpg	336.89	J/molxK	645.27	Joback Method
cpg	346.39	J/molxK	678.07	Joback Method
dvisc	0.0080597	Paxs	259.27	Joback Method
dvisc	0.0034176	Paxs	296.27	Joback Method

dvisc	0.0017534	Paxs	333.28	Joback Method
dvisc	0.0010279	Paxs	370.28	Joback Method
dvisc	0.0006640	Paxs	407.29	Joback Method
dvisc	0.0004613	Paxs	444.29	Joback Method
dvisc	0.0003390	Paxs	481.30	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=C1482015&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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